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Some mathematical results on a system of transport equations with an algebraic constraint describing fixed-bed adsorption of gases

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Abstract

This paper deals with a system of two equations which describes heatless adsorption of a gaseous mixture with two species. When one of the components is inert, we obtain an existence result of a weak solution satisfying some entropy condition under some simplifying assumptions. The proposed method makes use of a Godunov-type scheme. Uniqueness is proved in the class of piecewise $\mathcal{C}^1$ functions.
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1. Introduction

Heatless adsorption is a cyclic process for the separation of a gaseous mixture, called "Pressure Swing Adsorption" cycle. During this process, each of the d species ($d \geqslant 2$) simultaneously exists under two phases, a gaseous and movable one with concentration $c_i(t, x)$ ($0 \leqslant c_i \leqslant 1$), or a solid (adsorbed) other with concentration $q_i(t, x)$, $1 \leqslant i \leqslant d$. Following Ruthwen (see [12] for a precise description of the process), we can describe the evolution of u, c_i, q_i according to the following system, where $C = (c_1, \ldots, c_d)$:

$$\partial_t c_i + \partial_x(uc_i) = A_i(q_i - q_i^*)(C), \tag{1}$$

$$\partial_t q_i + A_i q_i = A_i q_i^*(C), \quad t \geqslant 0, \ x \in (0, 1), \tag{2}$$

with suitable initial and boundary data. In (1)–(2) the velocity $u(t, x)$ of the mixture has to be found in order to achieve a given pressure (or density in this isothermal model)

$$\sum_{i=1}^{d} c_i = \rho(t), \tag{3}$$

where ρ represents the given total density of the mixture. The experimental device is realized so that it is a given function depending only upon time. The function q_i^* is defined on $(\mathbb{R}_+)^d$, depends upon the assumed model and represents the equilibrium concentrations. Its precise form is usually unknown but is experimentally obtained. Simple examples of such a function are for instance the linear isotherm $q_i^* = K_i c_i$, with $K_i \geqslant 0$ and the Langmuir isotherm $q_i^* = (Q_i K_i c_i)/(1 + \sum_{j=1}^{d} K_j c_j)$, with $K_i \geqslant 0$, $Q_i > 0$ (see, for instance, [2,7,12]).

The right-hand side of (1)–(2) rules the matter exchange between the two phases and quantifies the attraction of the system to the equilibrium state: it is a pulling back force and A_i is the "velocity" of exchange for the species i. A component with concentration c_k is said to be inert if $A_k = 0$ and $q_k = 0$.

A theoretical study of the system (1)–(3) was presented in [1] and a numerical approach was developed in [2]. Let us point out that one of the mathematical interests of the above model is its analogies and differences compared to various other classical equations of physics or chemistry. First, when $d = 1$ (and eventually with $A_i = 0$) this model shares a similar structure with conservation laws under the form

$$\partial_t \rho + \partial_x\big(\rho u(\rho)\big) = 0, \qquad \partial_x u(\rho) = F(\rho),$$

where $u(\rho)$ has an integral dependance upon ρ, while in scalar conservation laws u depends upon ρ. In [1] both BV and L^∞ theories are developed for this model, but oscillations can propagate thus differing from Burger's example (see Tartar [15], Lions et al. [10]).

Secondly, when the coefficients A_i tend to infinity (instantaneous equilibrium), we get formally

$$q_i - q_i^* = -\frac{1}{A_i} \partial_t q_i \to 0$$

and Eqs. (1)–(2) reduce to

$$\partial_t\big(c_i + q_i^*(C)\big) + \partial_x(uc_i) = 0, \quad i = 1, \dots, d. \tag{4}$$

Joined to (3), the system of conservation laws (4) generalizes the system of chromatography which has been intensively studied (see [6,11] for the Langmuir isotherm) whereas the system (1)–(2) enters more in the field of relaxation systems (see, for instance, Jin and Xin [8], Katsoulakis and Tzavaras [9]). Actually the system of chromatography corresponds, like in (4), to instantaneous adsorption, but the fluid speed is a constant $u(t, x) = u$. One may consult James [6] for a numerical analysis and the relationships with thermodynamics, Canon and James [3] in the case of the Langmuir isotherm. In [7], James studied a system closely related to (1)–(2) in which the speed is constant and the coefficients A_i are equal to $1/\varepsilon$, where ε is a small parameter. Using compensated compactness, he proved, under some assumptions on the flux, that the solution of this system converges, as $\varepsilon \to 0$, to a solution of a system of quasilinear equations similar

to (4) satisfying a set of entropy inequalities. The extension of his method to (4) with constraint (3) seems not straightforward and is still an open problem.

In this paper, we deal with the system of equations (4)–(3) with two components ($d = 2$), one adsorbable with concentration c_1 and one inert with concentration c_2. Moreover, in (3) we assume that $\rho \equiv 1$, which is not really restrictive from a theoretical point of view. Then, the corresponding system of transport equations writes:

$$\partial_t\big(c_1 + q_1^*(c_1, c_2)\big) + \partial_x(uc_1) = 0, \tag{5}$$
$$\partial_t c_2 + \partial_x(uc_2) = 0, \tag{6}$$

with the algebraic constraint

$$c_1 + c_2 = 1. \tag{7}$$

Notice that we seek positive solutions (c_1, c_2), thus, in view of (7), c_1, c_2 must satisfy $0 \leqslant c_1, c_2 \leqslant 1$. Adding (5) and (6), we get, thanks to (7):

$$\partial_t q_1^*(c_1, c_2) + \partial_x u = 0.$$

In the sequel we set $c := c_2$ and $h(c) = -q_1^*(c_1, c_2) = -q_1^*(1 - c, c)$, thus our purpose is to study the system (5)–(7) under the form:

$$\begin{cases} \partial_t c + \partial_x(uc) = 0, \\ \partial_t h(c) - \partial_x u = 0, \end{cases} \tag{8}$$

supplemented by initial and boundary values:

$$\begin{cases} c(0, x) = c_0(x) \in [0, 1], & x > 0, \\ c(t, 0) = c_b(t) \in [0, 1], & t > 0, \\ u(t, 0) = u_b(t), & t > 0. \end{cases} \tag{9}$$

We assume in (9) an influx boundary condition, i.e., $\forall t > 0$, $u_b(t) > 0$. We choose $]0, +\infty[$ instead of $]0, 1[$ as spatial domain for the sake of simplicity. In order to investigate some properties of the function h, we look at some commonly used isotherm [16]. For linear isotherm, we have: $q_1^* := K_1 c_1$ with $K_1 > 0$, then

$$h'(c) := \frac{dh}{dc} > 0 \tag{10}$$

and $h'' = 0$. For the binary Langmuir isotherm which is: $q_1^* = (Q_1 K_1 c_1)/(1 + K_1 c_1 + K_2 c_2)$, with $K_1 > 0$, $Q_1 > 0$, $K_2 \geqslant 0$, we have also $h' > 0$, and $h''(c) := \frac{d^2 h}{dc^2} \geqslant 0$ if $K_2 < K_1$ (actually $K_2 = 0$ if the second species is inert). For the so-called BET isotherm defined by

$$q_1^* = \frac{QKc_1}{(1 + Kc_1 - (c_1/c_s))(1 - (c_1/c_s))}, \quad Q > 0, \ K > 0, \ c_s > 0,$$

we have still $h' > 0$ but no longer $h'' \geqslant 0$. Nevertheless the function $h' + ch''$, first derivative of $H(c) := 1 + ch'(c)$ remains nonnegative for a convenient choice of the parameters (but unfortunately not in all the physically relevant situations). In this first simplified approach we will assume (10) and

$$H'(c) \geqslant 0. \tag{11}$$

Single-component adsorption is of course of a poor physical meaning, but must be understood as a preliminary theoretical study.

The paper is organized as follows. In Section 2, we give some results for smooth solutions. These results suggest us an entropy condition. In Section 3, we give solutions for the Riemann problem satisfying such an entropy condition. In Section 4, we use a Godunov scheme to construct an approximate weak solution of problem (8)–(9) and we give some useful bounds. Next, in Section 5, we obtain an existence theorem for a weak solution of problem (8)–(9). Lastly, in Section 6, the uniqueness is obtained in the class on piecewise $\mathcal{C}^1$ functions.

2. Smooth solutions

Proposition 2.1. *For smooth solutions, the system* (8) *with the initial boundary conditions* (9) *becomes*:

$$\partial_t c + \partial_x\big[\alpha(t)F(c)\big] = 0, \quad t, x > 0, \tag{12}$$

$$c(0, x) = c_0(x), \quad x > 0, \tag{13}$$

$$c(t, 0) = c_b(t), \quad t > 0, \tag{14}$$

with $\alpha(t) = u_b(t)\exp(g(c_b(t))) > 0$, $F(c) = c\exp(-g(c)) > 0$, where

$$g'(c) = \frac{h'(c)}{H(c)}, \qquad H(c) = 1 + ch'(c) \tag{15}$$

and necessarily

$$u(t, x) = \alpha(t)\exp\big(-g\big(c(t, x)\big)\big) > 0, \quad t, x > 0. \tag{16}$$

Moreover, under assumption (10)–(11) *we have $F' > 0 > F''$.*

Notice that g and F depend only on h', but α depends also on boundaries values u_b, c_b. The maximum principle is valid for c but not for u: see, for instance, Fig. 6.

Proof. Since c and u are smooth, we can apply the chain rule formula. So, the second equation of (8) can be rewritten $\partial_x u = h'(c)\partial_t c$, then, with the first equation, $\partial_x u = -h'(c)\partial_x(uc)$ and we get $(\partial_x u)(1 + ch'(c)) = -uh'(c)\partial_x c$. Finally, with the notations introduced in (15) we have:

$$\partial_x u = -uh'(c)(\partial_x c)/H(c) = -u\partial_x\big(g(c)\big). \tag{17}$$

For a fixed $t > 0$, the function $x \mapsto u(t, x)$ is the unique solution of the ordinary linear differential equation (17) with the "initial" condition $u(t, 0) = u_b(t) > 0$. Explicitly, we have: $u(t, x) = u_b(t)\exp(g(c_b(t)) - g(c(t, x)))$, then $u(t, x)$ is positive for all x. Replacing u in the first equation of (8), we get (12). Now, a direct computation gives us:

$$F'(c) = \exp\big(-g(c)\big)/H(c), \qquad F''(c) = -\frac{\exp(-g(c))}{H^2(c)}\big(H'(c) + h'(c)\big) \tag{18}$$

and thanks to the hypothesis (10) and (11) we have $F' > 0$ and $F'' < 0$: the flux in the scalar conservation law (12) is strictly concave. $\square$

Theorem 2.1 (Global smooth solution). *Assume* (10)–(11).
If $u_b \in C^1([0, +\infty[,]0, +\infty[)$, if $c_b, c_0 \in C^1([0, +\infty[, [0, 1])$ satisfy the following compatibility conditions at the corner:

$$c_b(0) = c_0(0), \qquad c'_b(0) + u_b(0)c'_0(0) + h'\big(c_b(0)\big)c'_b(0)c_0(0) = 0$$

and if $c_0' \leqslant 0 \leqslant c_b'$, then the system (8)–(9) admits one and only one smooth solution:

$$(c, u) \in C^1\big([0, +\infty[_t \times [0, +\infty[_x, [0, 1]\big) \times C^1\big([0, +\infty[_t \times [0, +\infty[_x,]0, +\infty[\big).$$

Moreover: $\forall t > 0$, $\partial_x c(t, x) \leqslant 0$, $u(t, x) > 0$, $\partial_x u(t, x) \geqslant 0$.

We deduce from this result an entropy condition for shock waves:

(EC) "*c increases through a shock.*"

For smooth solutions, the active gas desorbs and u increases to evacuate gases. Notice that the same theorem is true for continuous solutions with only one compatibility condition at the corner: $c_b(0) = c_0(0)$ and replacing the sign of the derivative of the concentrations on the boundary by monotonicity conditions. Figure 5 shows a (nonglobal) smooth solution which produces a shock wave in finite time.

Proof. For a smooth solution we can use the last proposition, so $\partial_t c + \alpha(t) F'(c) \partial_x c = 0$. Using the characteristic curve defined by

$$\frac{\partial X}{\partial s}(s, t, x) = \alpha(s) F'\big(c\big(s, X(s, t, x)\big)\big), \qquad X(t, t, x) = x, \tag{19}$$

we get

$$\frac{\partial}{\partial s} c\big(s, X(s, t, x)\big) = 0. \tag{20}$$

Thus, c is constant along the characteristic curve (19), i.e., $c(s, X(s, t, x)) = c(t, x)$, and X writes:

$$X(s, t, x) = x + F'\big(c(t, x)\big) \int_t^s \alpha(z) \, dz. \tag{21}$$

To construct a solution, we need only to construct all characteristic curves issuing from the boundary and verify that no characteristic curves cross each other, see [14, pp. 241–244] or [5], i.e., we need to satisfy: $\beta := \partial_x X(s, t, x) > 0$. Differentiating (19) with respect to x, we get

$$\frac{\partial \beta}{\partial s}(s, t, x) = \alpha(s) F''\big(c\big(s, X(s, t, x)\big)\big) \partial_x c\big(s, X(s, t, x)\beta, \qquad \beta(t, t, x) = 1.$$

On the other hand, we have $\partial_x c(s, X(s, t, x)) = \partial_x c(t, x)$, then for $s > t$:

$$\frac{\partial \beta}{\partial s}(s, t, x) = \big[\alpha(s) \times F''\big(c(t, x)\big) \times \partial_x c(t, x)\big] \beta(s, t, x), \qquad \beta(t, t, x) = 1.$$

Since $F''(c) < 0$ and $\alpha(s) > 0$, the sufficient way to keep β positive is: $\forall (t, x)$, $\partial_x c(t, x) \leqslant 0$. Since $\partial_x c$ is constant along any characteristic curve, it suffices to satisfy this condition on the boundary. For characteristic curves issuing from $\{t = 0\}$, this last condition becomes $\partial_x c(0, x) = c_0'(x) \leqslant 0$. For characteristic curves issuing from $\{x = 0\}$, remark that on $x = 0$, thanks to Eq. (12), we have $\partial_t c(t, 0) = -\alpha(t) F'(c(t, 0)) \partial_x c(t, 0)$. Since $F'(c) > 0$ and $\alpha(t) > 0$ we need to have $\partial_t c(t, 0) = c_b'(t) > 0$. $\quad \square$

3. Riemann problem

It is well known (see, for instance, Dafermos [4], Serre [13], Smoller [14]) that in the context of hyperbolic systems of conservation laws, the life span of smooth solutions is finite even when the initial/boundary data are smooth. For the system studied in this paper, it will be the case if for instance the monotonicity conditions $c'_0 \leqslant 0 \leqslant c'_b$ are not satisfied, thus we have to deal with weak solutions. In order to get a general existence result via the construction of a sequence of approximate solutions, we are going to adapt the Godunov scheme to the system (8): the first step is the resolution of the Riemann problem.

We are thus looking for a weak solution of the following Riemann problem:

$$\partial_t c + \partial_x(uc) = 0, \qquad \partial_t h(c) - \partial_x u = 0,$$
$$\forall x > 0, \quad c(0, x) = c_+,$$
$$\forall t > 0, \quad c(t, 0) = c_- \quad \text{and} \quad u(t, 0) = u_-, \tag{22}$$

with $c_-, c_+ \in [0, 1]$ and $u_- > 0$. By symmetry, we search a selfsimilar solution, i.e.: $c(t, x) = C(z)$, $u(t, x) = U(z)$ with $z = \frac{x}{t} > 0$. Recall that from Theorem 2.1 we proposed the following (EC) entropy condition for shock waves: c increases through a shock. Then, if $c_- > c_+$, we find a continuous solution. To have a global smooth solution, we find necessarily a decreasing solution thanks to Theorem 2.1 and if $c_- < c_+$, we find a shock wave.

Proposition 3.1 (Rarefaction wave). *Assume* (10)–(11). *If* $c_- > c_+$, *the only smooth selfsimilar solution of* (22) *is such that*

$$\begin{cases} C(z) = c_-, & 0 < z < z_-, \\ \frac{dC}{dz} = -\frac{G(C)}{z}, & z_- < z < z_+, \\ C(z) = c_+, & z_+ < z, \end{cases} \tag{23}$$

where

$$G(c) = \frac{H(c)}{h'(c) + H'(c)} > 0, \qquad z_- = \frac{u_-}{H(c_-)} > 0, \tag{24}$$

z_+ *is defined by the equation* $C(z_+) = c_+$, $u_+ = z_+ H(c_+)$, *and* U *is given by*

$$\begin{cases} U(z) = u_-, & 0 < z < z_-, \\ U(z) = zH(C(z)), & z_- < z < z_+, \\ U(z) = u_+, & z_+ < z. \end{cases} \tag{25}$$

So, along a rarefaction wave, c decreases, u increases, $z_- < u_-$, and $z_+ < u_+$. Notice that the computations of z_+ and u_+ need the resolution of an ODE. Figure 2 shows a desorption step corresponding to a rarefaction wave arising from a discontinuity at $(t = 0, x = 0)$.

Proof. Setting $C'(z) = \frac{dC}{dz}$ and $U'(z) = \frac{dU}{dz}$, we get from (8)

$$-zC' + (UC)' = 0, \tag{26}$$
$$U' = -zh'(C)C'. \tag{27}$$

Using Eq. (27), we get $UC' = zH(C)C'$, so, where $C' \neq 0$:

$$U(z) = zH\big(C(z)\big). \tag{28}$$

We are looking for a simple wave, so $C' \neq 0$ on (z_-, z_+). From (28), z_- is defined by $z_- = u_-/H(c_-)$ and we have to find z_+ and u_+.

From (28) and (26) we get $\frac{C'(z)}{G(C)} = -\frac{1}{z}$. Let $\phi(C) = \int_{c_-}^{C} \frac{1}{G(s)} ds$. Thanks to the hypothesis (10)–(11) we have $G > 0$ and, for $C < c_-$, we have $\phi(C) < 0$. But $\frac{d}{dz}\phi(C(z)) = \phi'(C)C'(z) = \frac{C'(z)}{G(C)} = -\frac{1}{z}$. Then $\phi(C(z)) = \ln(\frac{z_-}{z})$ because $\phi(c_-) = 0$. Finally, $\phi(C(z_+)) = \ln(\frac{z_-}{z_+})$ and $z_+ = z_- \exp(-\phi(c_+))$. Now, using again (28), we get u_+. $\square$

Proposition 3.2 (Shock wave). *Assume* (10)–(11). *If* $c_- < c_+$, *the only weak selfsimilar solution of* (22) *is*

$$C(z) = \begin{cases} c_- & \text{if } 0 < z < s, \\ c_+ & \text{if } s < z, \end{cases} \qquad U(z) = \begin{cases} u_- & \text{if } 0 < z < s, \\ u_+ & \text{if } s < z, \end{cases} \tag{29}$$

where u_+ *is defined by*

$$u_+ = u_- \frac{[c] + c_-[h]}{[c] + c_+[h]}, \tag{30}$$

and where the speed s *of the shock satisfies*

$$0 < s = -\frac{[u]}{[h]} = \frac{[uc]}{[c]} = u_- \frac{[c]}{[c] + c_+[h]} = u_+ \frac{[c]}{[c] + c_-[h]} < u_+ < u_- \tag{31}$$

with the classical notations for the jumps.

Thanks to the Rankine–Hugoniot condition, this is the only weak monotonic solution with only one jump, i.e., c and u are monotonic functions. So, through a shock wave, c increases, u decreases but remains positive. The speed of the shock is proportional to u_- and lower than the fluid velocity u. Notice the difference with a strictly hyperbolic 2×2 system. Here we have three data: c_-, c_+, u_- and two unknowns: u_+, s. In the hyperbolic case for two shocks, we have four data: c_-, c_+, u_-, u_+ and four unknowns: c_0, u_0, s_1, s_2. Figure 3 shows an adsorption step corresponding to a shock wave arising from a discontinuity at $(t = 0, x = 0)$. See also Fig. 4 for the junction of two shocks.

Proof. We cannot find a smooth solution since $G > 0$ and c should decrease, by (23). Let be $\nu = (\nu_t, \nu_x)$ a normal vector to the shock line. The Rankine–Hugoniot conditions write $\nu_t[c] + \nu_x[uc] = 0$, $\nu_x[u] = \nu_t[h(c)]$. We have $[c] \neq 0$ thus $[h(c)] \neq 0$ and $\nu_x \neq 0$. Then the slope s of the shock line satisfies $s = [uc]/[c] = -[u]/[h]$. Then from $[u][c] + [uc][h] = 0$ we get

$$\frac{u_+}{u_-} = \frac{[c] + c_-[h]}{[c] + c_+[h]} \tag{32}$$

and all results follow. $\square$

Remark 3.1. For the Riemann problem notice that c satisfies the maximum principle. It is very important since c must be in $[0, 1]$. Notice also that for all $t > 0$ the functions $c(t, \cdot)$ and $u(t, \cdot)$ are monotonic thanks to (10)–(11).

Lemma 3.1. *Assume* (10)–(11). *For the solution of the Riemann problem* (22) *given in Propositions* 3.1 *and* 3.2 *we have the following estimate*:

$$\left|\ln(u_+) - \ln(u_-)\right| \leqslant \gamma |c_+ - c_-|,$$

where γ *is a true constant depending only on the* h *function.*

Proof. If the solution of the Riemann problem (22) is a rarefaction wave then, by Proposition 3.1, we have: $0 < \frac{u_+}{u_-} = \frac{z_+ H(c_+)}{z_- H(c_-)} < \frac{z_+}{z_-}$, since $c_- > c_+$ and $c \mapsto H(c)$ is an increasing function. Let be $\beta = \min_{0 \leqslant c \leqslant 1} G(c) > 0$ and D the upper solution: $\frac{dD}{dz} = -\frac{\beta}{z}$, $z_- \leqslant z < z_+$, $D(z_-) = c_-$, $C(z) \leqslant D(z)$ on (z_-, z_+). Let be z_0 determined by $D(z_0) = c_+$: necessarily $z_+ \leqslant z_0$. We can compute explicitly D and z_0: $D(z) = c_- - \beta \ln(z/z_-)$, $z_0 = z_- \exp(|c_+ - c_-|/\beta)$. Then, it suffices to take $\gamma_1 = \frac{1}{\beta} = \frac{1}{\min_{c \in [0,1]} G(c)}$. If the solution of the Riemann problem (22) is a shock wave then, by Proposition 3.2 and equality (32), we have:

$$0 < \frac{u_+}{u_-} = \frac{[c] + c_-[h]}{[c] + c_+[h]} = S(c_-, c_+), \quad c_- < c_+.$$

The function S is smooth and positive on $\Omega = \{(c_-, c_+), \ 0 \leqslant c_- < c_+ \leqslant 1\}$. On the diagonal we have $c_- = c_+$ and $S \equiv 1$, therefore we verify that $\ln(S)$ is a smooth function on $\overline{\Omega}$, vanishing on the diagonal. Then, there exists γ_2 such that $|\ln(u_+) - \ln(u_-)| \leqslant \gamma_2 |c_+ - c_-|$. Finally Lemma 3.1 holds with $\gamma = \max(\gamma_1, \gamma_2)$. $\quad \square$

4. Godunov scheme

We adapt the classical Godunov scheme for hyperbolic systems to the system of adsorption (8). Let be $T > 0$, $X > 0$ fixed. For a fixed integer N we set $\Delta x = \frac{X}{N+1}$ and $\Delta t = \frac{T}{M+1}$, where M is an integer depending upon N and will be chosen later to satisfy a CFL-type condition. We are going to build an approximate solution (c^N, u^N) of (8) on $(0, T) \times (0, X)$. For $i = 0, \ldots, N$ and $j = 0, \ldots, M$ we denote by $B_{i,j}$ the box $B_{i,j} = [t_j, t_{j+1}[\times [x_i, x_{i+1}[$, where $x_i = i\Delta x$, $t_j = j\Delta t$. We use also middle mesh ($x_{i+1/2} = x_i + \Delta x/2$, $t_{j+1/2} = t_j + \Delta t/2$). We discretize the initial boundary values as follows:

$$c^N(0, x) = c^N(0, x_{i+1/2}) := \frac{1}{\Delta x} \int_{x_i}^{x_{i+1}} c_0(x)\, dx, \quad x_i < x < x_{i+1},$$

$$c^N(t, 0) = c^N(t_{j+1/2}, 0) := \frac{1}{\Delta t} \int_{t_j}^{t_{j+1}} c_b(t)\, dt, \quad t_j < t < t_{j+1},$$

$$u^N(t, 0) = u^N(t_{j+1/2}, 0) := \frac{1}{\Delta t} \int_{t_j}^{t_{j+1}} u_b(t)\, dt, \quad t_j < t < t_{j+1},$$

where $0 \leqslant i \leqslant N$ and $0 \leqslant j \leqslant M$. For the Godunov scheme we need a CFL condition: solving a Riemann problem on the box $B = [0, \Delta t[\times [0, \Delta x[$ with the initial value c^+ and the boundary values c^-, u^- (on $\{x = 0\}$), we want that the wave leaves the box B by its upper side $\{\Delta t\} \times [0, \Delta x[$, i.e., $z_+ \Delta t < \Delta x$ for a rarefaction wave and $s \Delta t < \Delta x$ for a shock. Since $z_+ < \max(u_-, u_+)$ or $s < \max(u_-, u_+)$, this is clearly satisfied under the following (CFL) condition:

$$\sup_{[0, \Delta t[\times [0, \Delta x[} u = \max(u_-, u_+) < \frac{\Delta x}{\Delta t}. \tag{33}$$

If this CFL condition is always satisfied, we can compute (c^N, u^N) row by row (i.e., for each fixed j) solving the Riemann problem on each box $B_{i,j}$, $i = 0, \ldots, N$, according to the following procedure.
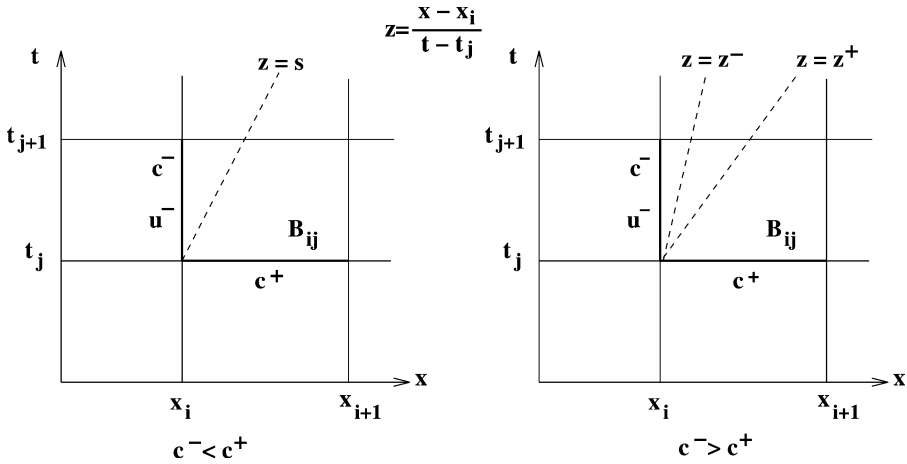
$$z = \frac{x - x_i}{t - t_j}$$

Fig. 1. Riemann problem in a box B_{ij}.

Assume that, for a given i, we have given $c^N(t_j, x) = c^+$ on $[x_i, x_{i+1}[$, $c^N(t, x_i) = c^-$ and $u^N(t, x_i) = u^-$ on $[t_j, t_{j+1}[$, then:

(1) if $c^- < c^+$ (shock) we compute s and u^+ according to (31) and (30). Thanks to the CFL condition and (29) we get $c^N(t, x_{i+1}) = c^+$, $u^N(t, x_{i+1}) = u^+$ on $[t_j, t_{j+1}[$ and we define $c^N(t_{j+1}, x)$ on $[x_i, x_{i+1}[$ as the mean value of the solution of the Riemann problem, that is:

$$c^N(t_{j+1}, x) = c^N(t_{j+1}, x_{i+1/2}) := \lambda s c^- + (1 - \lambda s)c^+ \quad \text{with } \lambda = \frac{\Delta t}{\Delta x};$$

(2) if $c^- > c^+$ (rarefaction wave) we compute z^- by (24). Then, z^+ is computed as the unique solution of $C(z^+) = c^+$ with C defined through (23). U is defined by (25) with $u^+ = z^+ H(z^+)$. As in the preceding case we have $c^N(t, x_{i+1}) = c^+$, $u^N(t, x_{i+1}) = u^+$ on $[t_j, t_{j+1}[$ and we define $c^N(t_{j+1}, x)$ on $[x_i, x_{i+1}[$ as the mean value of the solution of the Riemann problem. Using for instance the trapezoid rule we get:

$$c^N(t_{j+1}, x) = c^N(t_{j+1}, x_{i+1/2}) := \lambda \frac{z^- + z^+}{2} c^- + \left(1 - \lambda \frac{z^- + z^+}{2}\right) c^+.$$

Notice that we could proceed as well by columns before rows (i before j). To ensure the CFL condition (33), we need to control $\sup u$. Therefore, by Lemma 3.1, we have to control the total variation in space of c for all time. Recall that, for any function v defined on (a, b):

$$TV(v, (a, b)) = \sup\left\{\sum_{k=0}^{n}|v(z_{k+1}) - v(z_k)|; \ n \in \mathbb{N}, \ a < z_0 < \cdots < z_{n+1} < b\right\}$$

$$= \sup\left\{\left|\int_a^b v(z)\phi'(z)\,dz\right|; \ \phi \in C_c^\infty(a, b), \ |\phi| \leqslant 1\right\}$$

and $v \in BV(a, b)$ if and only if $TV(v, (a, b)) < +\infty$.

In the following lemmas, we prove that this scheme is well defined and we give some useful bounds.

Lemma 4.1. *Let be γ the constant defined in Lemma* 3.1. *If the CFL condition is fulfilled, then, for all $t \in (0, T)$:*

$$TV\big[\ln\big(u(t, .)\big), (0, X)\big] \leqslant \gamma TV\big[c(t, .), (0, X)\big].$$

Proof. This is a direct application of Lemma 3.1, the algorithm of Godunov scheme and the monotonicity of c and u on each box (see Remark 3.1). □

Let us define the total variation of initial-boundary concentration by

$$TV(c_b, c_0) := TV\big(c_b, (0, T)\big) + TV\big(c_0, (0, X)\big) + \sup_{0 < t < T,\, 0 < x < X} \big|c_b(t) - c_0(x)\big|. \tag{34}$$

Lemma 4.2. *If the CFL condition is fulfilled, then, for all $N \geqslant 0$:*

$$\sup_{0 < t < T} TV\big[c^N(t, .), (0, X)\big] \leqslant TV(c_b, c_0).$$

Proof. By monotonicity of the solution of the Riemann problem under the CFL condition (see Remark 3.1) we have, for all $t \in (t_j, t_{j+1})$ and all $t \in (t_j, t_{j+1})$:

$$TV\big[c^N(t, .), (x_i, x_{i+1})\big] = \big|c^N(t_{j+1/2}, x_i) - c^N(t_{j+1/2}, x_{i+1})\big|.$$

Therefore, we have:

$$TV\big[c^N(t_{j+1/2}, .), (0, X)\big] = \sum_{i=0}^{N} \big|c^N(t_{j+1/2}, x_{i+1}) - c^N(t_{j+1/2}, x_i)\big|.$$

In particular, in the lower row, we obtain:

$$\begin{aligned}
TV\big[c^N(t_{1/2}, .), (0, X)\big] &= \big|c^N(t_{1/2}, 0) - c^N(0, x_{1/2})\big| \\
&\quad + \sum_{i=1}^{N} \big|c^N(0, x_{i-1/2}) - c^N(0, x_{i+1/2})\big| \\
&\leqslant \big|c^N(t_{1/2}, 0) - c^N(0, x_{1/2})\big| + TV\big(c_0(.), (0, X)\big).
\end{aligned}$$

By induction, we get easily

$$TV\big[c^N(t_{j+1/2}, .), (0, X)\big] \leqslant \big|c^N(t_{j+1/2}, 0) - c^N(t_j, x_{1/2})\big| + TV\big[c^N(t_{j-1/2}, .), (0, X)\big].$$

Since $c^N(t_j, x_{1/2})$ is between $c^N(t_{j-1/2}, 0)$ and $c^N(t_{j-1}, x_{1/2})$ we have

$$\begin{aligned}
\big|c^N(t_{j+1/2}, 0) - c^N(t_j, x_{1/2})\big| &\leqslant \big|c^N(t_{j+1/2}, 0) - c^N(t_{j-1/2}, 0)\big| \\
&\quad + \big|c^N(t_{j-1/2}, 0) - c^N(t_{j-1}, x_{1/2})\big|.
\end{aligned}$$

Then, we get

$$\begin{aligned}
&TV\big[c^N(t_{j+1/2}, .), (0, X)\big] \\
&\qquad \leqslant \sum_{k=1}^{j} \big|c^N(t_{k+1/2}, 0) - c^N(t_{k-1/2}, 0)\big| + TV\big[c^N(\Delta t/2, .), (0, X)\big]
\end{aligned}$$

$$\leqslant \sum_{k=1}^{j} \left| c^N(t_{k+1/2}, 0) - c^N(t_{k-1/2}, 0) \right| + \left| c^N(t_{1/2}, 0) - c^N(0, x_{1/2}) \right|$$

$$+ TV\left(c_0(.), (0, X)\right)$$

$$\leqslant TV\left(c_b(.), (0, t_{j+1})\right) + \left| c^N(t_{1/2}, 0) - c^N(0, x_{1/2}) \right| + TV\left(c_0(.), (0, X)\right)$$

$$\leqslant TV(c_b, c_0). \quad \square$$

Lemma 4.3. *Let be* $\lambda = \|u_b\|_\infty \times \exp(\gamma TV(c_b, c_0)) > 0$. *If* $\lambda \Delta t < \Delta x$, *then the CFL condition is fulfilled.*

Proof. We proceed by induction. Let $(H_{i,j})$ the following hypothesis: on $R_{i,j} = (0, t_{j+1}) \times (0, x_{i+1})$ we have

$$0 < u \leqslant \sup_{0 < t < t_{j+1}} \left(u_b(t) \exp\left(\gamma TV\left[c(t, .), (0, x_{i+1})\right]\right)\right). \tag{35}$$

Since $\lambda \geqslant \|u_b\|_\infty$, $(H_{0,j})$ is satisfied for all j. We have to show that for j from 0 to M, if $(H_{i,j})$ is true and $i < N$ then $(H_{i+1,j})$ is also true. To this purpose we need only to prove that u satisfies inequality (35) on $B_{i+1,j}$.

If $(H_{i,j})$ is true, the CFL condition is fulfilled on rectangle $R_{i,j}$, then

$$u_- := u(t_{j+1/2}, x_{i+1}) \leqslant \sup_{0 < t < t_{j+1}} \left(u_b(t) \exp\left(\gamma TV\left[c(t, .), (0, x_{i+1})\right]\right)\right).$$

Solving the Riemann problem on $B_{i+1,j}$, we get $u_+ \leqslant u_- \exp(\gamma |c_+ - c_-|)$ thanks to Lemma 3.1. Then,

$$\sup_{B_{i+1,j}} u \leqslant \sup_{0 < t < t_{j+1}} \left(u_b(t) \exp\left(\gamma TV\left[c(t, .), (0, x_{i+1})\right]\right)\right) \times \exp(\gamma |c_+ - c_-|)$$

$$\leqslant \sup_{0 < t < t_{j+1}} \left(u_b(t) \exp\left(\gamma TV\left[c(t, .), (0, x_{i+2})\right]\right)\right).$$

Therefore, $(H_{i+1,j})$ is true. Finally, we have $u \leqslant \lambda = \|u_b\|_\infty \exp(\gamma TV(c_b, c_0))$ and the CFL condition holds. $\square$

Denote by $ceil(x)$ the lowest integer bigger than x. We can fix M as follows:

$$M = 1 + ceil\left(\frac{\lambda T}{\Delta x}\right) = 1 + ceil\left(\lambda \frac{T}{X}(N + 1)\right) \tag{36}$$

and the CFL condition is then satisfied. Notice that $M \Delta x \sim \lambda T$ and $\frac{\Delta x}{\Delta t} \to \lambda$ as $N \to \infty$.

Lemma 4.4. *Let be* $L > 0$, $f \in BV(0, L)$, $\overline{f} = \frac{1}{L} \int_0^L f(x)\,dx$, *or* $\overline{f} = \frac{f(0^+)+f(L^-)}{2}$, *then*

$$\int_0^L \left| f(x) - \overline{f} \right| dx \leqslant L \times TV\left(f, (0, L)\right).$$

We skip the proof of this rather classical lemma.

Lemma 4.5. *Let be* $\lambda_1 = \sup_{N \in \mathbb{N}} \frac{\Delta x}{\Delta t} < \infty$, *then for any* $0 \leqslant s < t < T$ *the sequence* (c^N) *satisfies*:

$$\int_0^X \left| c^N(t, x) - c^N(s, x) \right| dx \leqslant 2\lambda_1 TV(c_b, c_0)\big(|t - s| + 2\Delta t\big). \tag{37}$$

Proof. We recall that CFL condition is fulfilled. First, we work on $B_{i,j}$, $t_j \leqslant s_1 < s_2 < t_{j+1}$. By monotonicity with respect to time of c^N on each box, we have

$$
\begin{aligned}
\int_{x_i}^{x_{i+1}} \left| c^N(s_2, x) - c^N(s_1, x) \right| dx &\leqslant \int_{x_i}^{x_{i+1}} \left| c^N(t_{j+1}, x - 0) - c^N(t_j, x) \right| dx \\
&\leqslant \Delta x \left| c^N(t_{j+1}, x_i) - c^N(t_j, x_{i+1/2}) \right| \\
&= \Delta x \, TV\big(c^N(t_{j+1/2}, .), (x_i, x_{i+1})\big).
\end{aligned}
$$

Since $\Delta x \leqslant \lambda_1 \Delta t$, after summation with respect to i, we get

$$\int_0^X \left| c^N(s_2, x) - c^N(s_1, x) \right| dx \leqslant \Delta x \, TV\big(c^N(t_{j+1/2}, .), (0, X)\big) \leqslant \lambda_1 \Delta t \, TV(c_b, c_0).$$

Otherwise, on $t = t_j$, there is a jump, but by Lemma 4.4:

$$
\begin{aligned}
\int_{x_i}^{x_{i+1}} \left| c^N(t_j, x) - c^N(t_j - 0, x) \right| dx &= \int_{x_i}^{x_{i+1}} \left| c^N(t_j, x_{1/2}) - c^N(t_j - 0, x) \right| dx \\
&\leqslant \Delta x \, TV\big(c^N(t_{j+1/2}, .), (x_i, x_{i+1})\big).
\end{aligned}
$$

Summing over i, we get

$$\int_0^X \left| c^N(t_j, x) - c^N(t_j - 0, x) \right| dx \leqslant \Delta x \, TV\big(c^N(t_{j+1/2}, .), (0, X)\big) \leqslant \lambda_1 \Delta t \, TV(c_b, c_0).$$

For any $0 \leqslant s < t < T$, let be $j := \min\{i, s \leqslant t_i\}$, $k := \max\{l, t_{j+l} \leqslant t\}$, and $s \leqslant t_j < t_{j+1} < \cdots < t_{j+k} \leqslant t$. By convention $t_{-1} = 0$, so we have $|t_{j+k+1} - t_{j-1}| \leqslant |t - s| + 2\Delta t$ and

$$
\begin{aligned}
\int_0^X \left| c^N(t, x) - c^N(s, x) \right| dx &\leqslant \sum_{l=-1}^k \int_0^X \left| c^N(t_{j+l+1}, x) - c^N(t_{j+l}, x) \right| dx \\
&\leqslant 2\lambda_1 TV(c_b, c_0)\big(|t - s| + 2\Delta t\big). \qquad \square
\end{aligned}
$$

Lemma 4.6. *Assume that the CFL condition is fulfilled, that* $u_b \in L^\infty(0, T)$, $\inf_{0 < t < T} u_b(t) > 0$ *and that* c_0 *and* c_b *have bounded variations. Then the sequence* (u^N) *is bounded in* $L^\infty((0, T) \times (0, X))$ *and in* $L^\infty(0, T; BV(0, X))$. *Furthermore*: $\inf_N \inf_{(0,T) \times (0,X)} u^N > 0$ *and* $\sup_N \|u^N\|_\infty \leqslant \|u_b\|_\infty \exp(\gamma TV(c_b, c_0))$.

Proof. Solving the Riemann problem, $u_+ > 0$ follows from $u_- > 0$ and we have $u^N > 0$ on $(0, T) \times (0, X)$. If $u_b \in L^\infty(0, T)$ and if $\inf_{0 < t < T} u_b(t) > 0$ then $\ln(u_b) \in L^\infty$. Thanks to Lemmas 4.1 and 4.2, if c_0 and c_b have bounded variations, we have $\sup_N \sup_{0 < t < T} TV_x(\ln(u^N(t, .))) < +\infty$ and Lemma 4.6 holds. □

5. Convergence towards a weak solution

Theorem 5.1 (Global large weak solution). *Let be $X > 0$, $T > 0$. Assume* (10)–(11) *and that $c_0 \in BV(0, X)$, $c_b \in BV(0, T)$, $u_b \in L^\infty(0, T)$, satisfying $0 \leqslant c_0, c_b \leqslant 1$ and $\inf_{0 < t < T} u_b(t) > 0$. Then the system* (8)–(9) *admits a weak solution given by Godunov scheme. Furthermore, c and u satisfy*:

$$c \in L^\infty\big((0, T) \times (0, X)\big) \cap L^\infty\big((0, T); BV(0, X)\big), \tag{38}$$

$$c \in \mathrm{Lip}\big(0, T; L^1(0, X)\big), \tag{39}$$

$$c \in BV\big((0, T) \times (0, X)\big), \tag{40}$$

$$u \in L^\infty\big((0, T) \times (0, X)\big) \cap L^\infty\big((0, T); BV(0, X)\big), \tag{41}$$

with the following bounds:

$$\int_0^X c(t, x)\, dx \leqslant \int_0^X c_0(x)\, dx + \|u_b\|_\infty \int_0^t c_b(s)\, ds, \tag{42}$$

$$0 \leqslant \min(\inf c_b, \inf c_0) \leqslant c \leqslant \max(\sup c_b, \sup c_0) \leqslant 1, \tag{43}$$

$$\|c\|_{L^\infty((0,T), BV(0,X))} \leqslant TV(c_b, c_0), \tag{44}$$

$$\|u\|_{L^\infty((0,T) \times (0,X))} \leqslant \|u_b\|_\infty \exp\big(\gamma TV(c_b, c_0)\big), \tag{45}$$

$$\inf_{[0,T] \times [0,X]} u > 0. \tag{46}$$

(γ is the constant defined in Lemma 4.3 *and depending only on the h function.)*

Proof. Let be $(c^N, u^N)_N$ the sequence constructed in Section 4. We are going to prove that a subsequence of $(c^N, u^N)_N$ converges towards a weak solution (c, u) of (8)–(9), satisfying the estimates (38) to (46).

First step: Convergence of c^N, u^N, $u^N c^N$ up to a subsequence.

By Lemma 4.2, the sequence (c^N) is bounded in $L^\infty((0, T); BV(0, X))$. Furthermore, by Lemma 4.5, we obtain a classical compactness argument on (c^N) (see [14]). Then, up to a subsequence, (c^N) converges to c in $L^1((0, T) \times (0, X))$ and a.e. Then c satisfies the same bounds, i.e., (38), (39), (43) and (44) hold, in particular c verifies the maximum principle.

By Lemma 4.6, the sequence (u^N) is bounded in L^∞, then, up to a subsequence, (u^N) converges weakly to u in L^∞ *weak-⋆*. By the same lemma, the sequence $(\partial_x u^N)$ is bounded $L_t^\infty M_x^1$, dual from $L_t^1 C_x^0$, then there exists $v \in L_t^\infty M_x^1$ such that $(\partial_x u^N)$ converges weakly to v in $L_t^\infty M_x^1$ *weak-⋆*. But the weak limit is unique then $\partial_x u = v$ and $u \in L_t^\infty BV_x$. Furthermore we have $\|u\|_{L^\infty} \leqslant \liminf_N \|u^N\|_{L^\infty} < +\infty$, $\|u\|_{L_t^\infty BV_x} \leqslant \liminf_N \|u\|_{L_t^\infty BV_x}^N < +\infty$, $\inf u \geqslant \inf_N u^N > 0$ and (41), (45), (46) hold. Now, we can pass to the limit in the nonlinear term $u^N c^N$ because the sequence (u^N) converges weakly to u in L^∞ *weak-⋆* and the sequence (c^N) converges strongly to c in L^1.

Second step: We show that (c, u), obtained in the previous step is a weak solution of (8)–(9). Recall that (c, u) is a weak solution of (8)–(9) on $(0, T) \times (0, X)$ if and only if, for any smooth functions $\phi, \psi \in C_c^\infty((-\infty, T) \times (-\infty, X))$:

$$\int_0^T \int_0^X (c \partial_t \phi + (cu) \partial_x \phi)(t, x) \, dx \, dt + \int_0^X c_0(x)\phi(0, x) \, dx \tag{47}$$

$$+ \int_0^T u_b(t) c_b(t) \phi(t, 0) \, dt = 0, \tag{48}$$

$$\int_0^T \int_0^X (h(c) \partial_t \psi - u \partial_x \psi)(t, x) \, dx \, dt + \int_0^X h(c_0(x))\psi(0, x) \, dx \tag{49}$$

$$- \int_0^T u_b(t)\psi(t, 0) \, dt = 0. \tag{50}$$

We are going to prove that (c, u) satisfies (47). A similar proof works to obtain (49). By construction, (c^N, u^N) is a weak solution of (8) on each box $B_{i,j}$ and, thanks to the fulfilled CFL condition, is also a weak solution on each row $(t_j, t_{j+1}) \times (0, X)$. The problem is only on line $t = t_j, 0 < j \leqslant M$ and $t = 0, x = 0$ for the discretisation of the initial boundary value (9). So, for any ϕ, we have

$$\int_0^T \int_0^X (c^N \partial_t \phi + c^N u^N \partial_x \phi)(t, x) \, dx \, dt + \int_0^X c^N(0, x)\phi(0, x) \, dx$$

$$+ \int_0^T u^N(t, 0) c^N(t, 0)\phi(t, 0) \, dt = -J_N,$$

where $J_N = \sum_{j=1}^M \int_0^X (c^N(t_j, x + 0) - c^N(t_j, x - 0))\phi(t_j, x) \, dx$. In order to prove that (c, u) satisfies (47), thanks to the results of the first step, we have just to show that $J_N \to 0$. We can rewrite J_N under the form $J_N = \sum_{j=1}^M \sum_{i=0}^N J_{i,j}$ where

$$J_{i,j} = \int_0^{\Delta x} (\overline{c^N(t_j, x_{i+1/2})} - c^N(t_j, x_i + y))\phi(t_j, x_i + y) \, dy,$$

and

$$\overline{c^N(t_j, x_{i+1/2})} = \frac{1}{\Delta x} \int_0^{\Delta x} c^N(t_j, x_i + y) \, dy.$$

Since $\int_0^{\Delta x} (\overline{c^N(t_j, x_{i+1/2})} - c^N(t_j, x_i + y))\phi(t_j, x_i) \, dy = 0$, we write $\phi(t_j, x_i + y) = \phi(t_j, x_i) + (\phi(t_j, x_i + y) - \phi(t_j, x_i))$.

We have $|\phi(t_j, x_i + y) - \phi(t_j, x_i)| \leqslant \|\partial_x \phi\|_\infty \Delta x$ because $0 \leqslant y \leqslant \Delta x$. Thanks to Lemma 4.4, we have also

$$|J_{i,j}| = \left| \int\limits_0^{\Delta x} \overline{\left(c^N(t_j, x_{i+1/2}) - c^N(t_j, x_i + y)\right)} \left(\phi(t_j, x_i + y) - \phi(t_j, x_i)\right) dy \right|$$

$$\leqslant \|\partial_x \phi\|_\infty \Delta x \int\limits_0^{\Delta x} \left|\overline{c^N(t_j, x_{i+1/2}) - c^N(t_j, x_i + y)}\right| dy$$

$$\leqslant \|\partial_x \phi\|_\infty (\Delta x)^2 TV\big(c(t_j, .), (x_i, x_i + \Delta x)\big).$$

Therefore,

$$|J_N| \leqslant \sum_{j=1}^M \|\partial_x \phi\|_\infty (\Delta x)^2 TV\big(c^N(t_j, .), (0, X)\big) \leqslant \|\partial_x \phi\|_\infty TV(c_b, c_0) M \Delta x \times \Delta x$$

thus, if $M \leqslant \frac{T}{\Delta t}$, we have $|J_N| \leqslant T\|\partial_x \phi\|_\infty TV(c_b, c_0)\frac{\Delta x}{\Delta t} \times \Delta x$.

Since $\frac{\Delta x}{\Delta t} \to \lambda$ when $N \to \infty$, J_N converges towards 0. Lastly we get easily (42) by integrating (8) over $[0, t] \times [0, X]$ and using the positivity of u and c.

Last step: BV regularity of c.

Since (c, u) is a weak solution of (8) we have $\partial_x u = \partial_t h(c)$ and, thanks to the estimate on $\partial_x u$, we get $\partial_t h(c) \in L^\infty((0, T); M^1(0, X))$. We have $h' > 0$, then $c = h^{-1}(h(c))$ and the chain rule formula in BV gives $\partial_t c = (h^{-1})' \partial_t h(c) \in L^\infty M_x^1$. Then $\partial_t c$ and $\partial_x c$ lie in $M^1((0, T) \times (0, X))$ and finally $c \in BV((0, T) \times (0, X))$, which is (40). $\quad\square$

We have now strong trace results.

Proposition 5.1. *The functions c and u satisfy initial boundary conditions* (9) *strongly.*

Proof. The function c belongs to $BV((0, T) \times (0, X))$, then admits a strong trace on $\{t = 0\}$ and $\{x = 0\}$. But c is a weak solution of (8), (9), then admits also a weak trace on the boundary. By uniqueness of traces, c satisfies the initial boundary conditions (9) strongly. On the other hand, u belongs to $L^\infty((0, T) \times (0, X)) \cap L^\infty((0, T); BV(0, X))$, then admits a strong trace $v(t)$ in $\{x = 0\}$ defined for a.e. $t \in (0, T)$. We have $u(t, x) \to v(t)$ for a.e. t when $x \to 0^+$ and $v \in L^\infty(0, T)$ with $\|v\|_{L_t^\infty} \leqslant \|u\|_{L_{t,x}^\infty}$, thus, thanks to the Lebesgue's theorem, u admits v as strong trace on $\{x = 0\}$ in $L^1(0, T)$: $\lim_{x \to 0^+} \int_0^T |\tilde{u}(t, x) - v(t)| dt = 0$, where $\tilde{u}$ is defined for a.e. $t \in [0, T]$ and all $x \in [0, X]$ as the mean value $\tilde{u}(t, x) = \frac{u(t, x-0) + u(t, x+0)}{2}$. $\quad\square$

6. Uniqueness

We study the uniqueness problem for weak entropic solutions in some class of piecewise smooth functions. More precisely we denote by $\mathcal{C}_p^1([0, T] \times [0, X], \mathbb{R}^2)$ ($\mathcal{C}_p^1$ in brief) the set of functions $(c, u): [0, T] \times [0, X] \to \mathbb{R}^2$ such that there exists a finite number of continuous and piecewise $\mathcal{C}^1$ curves outside of which (c, u) is $\mathcal{C}^1$ and across which (c, u) has a jump discontinuity. In the sequel, we consider weak solutions $(c, u) \in \mathcal{C}_p^1$ of (8)–(9) in $(0, T) \times (0, X)$, with piecewise smooth initial and boundary data, satisfying the entropy condition (EC) and our usual assumptions (10)–(11) on h.

We restrict ourselves to the piecewise smooth case since we do not have a weak formulation for the entropy condition (EC). Formally we can expect to obtain such a condition as for hyperbolic PDEs, but it is still an open problem. Nevertheless, this case is relevant in most practical cases and involve global solutions with shock waves and contact discontinuities.

Theorem 6.1. *Let be T, $X > 0$. Let be $u_b : [0, T] \to \mathbb{R}_+$, $c_b : [0, T] \to [0, 1]$, $c_0 : [0, X] \to [0, 1]$ some piecewise $\mathcal{C}^1$ functions. Assume $\inf_{[0,T]} u_b(t) > 0$ and (10), (11). Then there exists at most one weak $\mathcal{C}_p^1$ solution (c, u) of the system (8)–(9) satisfying the entropy condition (EC), the maximum principle (43) and (46).*

Lemma 6.1. *Any shock curve across which c has a nonzero jump admits a parametrization $t \mapsto x(t)$.*

Proof. Let be $\nu = (\nu_t, \nu_x)$ a normal of the shock line. Since (c, u) is a weak solution, it satisfies the Rankine–Hugoniot condition and we get $\nu_x \neq 0$ and Lemma 6.1 holds. □

Remark. In the case where $[c] = 0$ and $[u] \neq 0$, the solution admits a contact discontinuity. We can easily obtain such a solution by considering for instance the following set of initial boundary data: $c_0 \equiv a$, $c_b \equiv a$, $u_b = u_1$ for $0 < t < t^*$ and $u_b = u_2$ for $t^* < t < T$. We have an obvious weak solution defined by $c(t, x) \equiv a$, $u(t, x) \equiv u_1$ on $(0, t^*) \times (0, X)$ and $u(t, x) \equiv u_2$ on $(t^*, T) \times (0, X)$: the boundary discontinuity of u is linearly propagated. Figure 6 shows an example of such a situation. We define now a "determination zone" $\Omega = \{(t, x), t_0 < t < t_1, x_1(t) < x < x_2(t)\}$ where $0 \leqslant t_0 < t_1 < T$, $x_1(t)$ and $x_2(t)$ are shock curves. We assume that $(c, u) \in \mathcal{C}^1(\Omega)$.

Lemma 6.2. *The characteristics curves lying in Ω satisfy*

$$0 < \frac{dX}{ds}(s, t, x) = \frac{u}{H(c)} \leqslant u. \tag{51}$$

Proof. Since $(c, u) \in \mathcal{C}^1(\Omega)$, we have $\partial_t c + \alpha(t) F'(c) \partial_x c = 0$, $u(t, x) = \alpha(t) \exp(-g(c(t, x)))$, where $\alpha(t) = (u \exp(g(c)))(t, x_1(t) + 0) = (u \exp(g(c)))(t, x_2(t) - 0) > 0$. Recall that the characteristics lines satisfy $\frac{dX}{ds}(s, t, x) = \alpha(s) F'(c(s, X(s, t, x)))$. Thanks to (16) and (18) we get immediately $\frac{dX}{ds}(s, t, x) = \frac{u}{H(c)}$. Since $h' > 0$, we have $H(c) = 1 + ch'(c) \geqslant 1$ and (51) holds. □

Lemma 6.3. *The forward characteristic lines enter the discontinuity (and the backward characteristic lines never enter a discontinuity).*

Proof. This proof relies on the entropy condition (EC). Let be $s \in]t_0, t_1[$ and $s \mapsto x(s)$ a shock curve. As usually we define $c_+ = c(s, x(s) + 0)$, $c_- = c(s, x(s) - 0)$, $u_+ = u(s, x(s) + 0)$ and $u_- = u(s, x(s) - 0)$. It follows from (19) that Lemma 6.3 reduces to the inequalities $\alpha(s) F'(c_+) < x'(s) < \alpha(s) F'(c_-)$. Consider for instance the fist one: thanks to (31) and (51) it is equivalent to $x'(s) = \frac{u_+[c]}{[c] + c_-[h]} > \frac{u_+}{H(c_+)}$. Now we have $u_+ > 0$, $c_+ > c_- > 0$, $H(c_+) = 1 + c_+ h'(c_+) > 0$ and the assumption (10), thus an easy computation leads to

$$\alpha(s) F'(c_+) < x'(s) \iff c_+ h'(c_+)[c] - c_-[h] > 0 \iff \phi(c_-) > 0,$$

where ϕ is defined by $\phi(y) = c_+ h'(c_+)(c_+ - y) - y(h(c_+) - h(y))$. We have

$$\phi'(y) = -\big(c_+ h'(c_+) - y h'(y)\big) - \big(h(c_+) - h(y)\big)$$
$$= -\big(H(c_+) - H(y)\big) - \big(h(c_+) - h(y)\big).$$

Thanks to (10) and (11) we have $\phi'(y) < 0$ for $y < c_+$, moreover $\phi(c_+) = 0$. Thus we get $\phi(c_-) > 0$ and Lemma 6.3 holds. $\quad\square$

Lemma 6.4. *From each point $(t_0, x_0) \in [0, T[\times [0, X[$ emerges at most one shock curve.*

Proof. Let be $(t_0, x_0) \in [0, T[\times [0, X[$ and assume that there exists two shock curves $x_1(s)$ and $x_2(s)$ issuing from (t_0, x_0) such that we have for instance $x_1(s) < x_2(s)$ locally in time $(t_0 < s < t_1)$ and (c, u) smooth in $Z := \{(s, \xi);\ t_0 < s < t_1,\ x_1(s) < \xi < x_2(s)\}$. Then we show easily that a backward characteristic line drawn from any point $(t, x) \in Z$ enter one of the two shock curves which contradicts Lemma 6.3. $\quad\square$

We prove now the local uniqueness for rarefaction waves.

Lemma 6.5. *Let be (t_0, x_0) a point of discontinuity for $c(t, x)$, $c_+ = c(t_0, x_0 + 0)$ and $c_- = c(t_0, x_0 - 0)$. If $c_- > c_+$, then there exists an open set $\mathcal{U}$ containing (t_0, x_0), there exists $t_1 > t_0$ such that (8)–(9) admits an unique smooth solution in $(]t_0, t_1[\times]0, X[) \cap \mathcal{U}$.*

Proof. We assume that $x_0 > 0$ (the case $x_0 = 0$ is similar). According to (EC) there is no shock curve passing through (t_0, x_0), thus the solution is smooth in an open set $\mathcal{V} =]t_0, t_1[\times]x_0 - 2\delta, x_0 + \delta[$ and has no discontinuity point in $\{t_0\} \times]x_0 - 2\delta, x_0[$ and in $\{t_0\} \times]x_0 + \delta[$. Let be $X_\pm$ the "limiting characteristics" defined for $s \geqslant t_0$, following (21), by $X_\pm(s) = x_0 + F'(c\pm) \int_{t_0}^{s} \alpha(\tau)\,d\tau$. We define as above the open set $Z = \{(s, \xi);\ t_0 < s < t_1,\ X_-(s) < \xi < X_+(s)\}$. Let be $(t, x) \in Z \cap \mathcal{V}$ and $X(s, t, x)$, $t_0 < s \leqslant t$, the associated backward characteristic line. We have $\lim_{s \to t_0 + 0} X(s, t, x) = x_0$ because the characteristic lines cannot cross each other, thus $x_0 = x - F'(c(t, x))A(t)$ with $A(t) = \int_{t_0}^{t} \alpha(s)\,ds$. Since F' is strictly decreasing (Proposition 2.1) we get $c(t, x) = (F')^{-1}(\frac{x - x_0}{A(t)})$ and conversely this last formula defines a smooth solution in Z. Along $(s, X_\pm(s))$ we have $c = c_\pm$ and $u = u_\pm$. Lastly the solution is defined in an unique way, using the characteristics lines, in $\mathcal{V} \cap \{X(s, t_0, x_0 - \delta) < x < X_-(s)\ \text{or}\ x > X_+(s)\}$ and Lemma 6.5 follows. $\quad\square$

We prove now the local uniqueness for the shock waves.

Lemma 6.6. *Let be $(t_0, x_0) \in [0, T[\times [0, X[$, $c_\pm = c(t_0, x_0 \pm 0)$ and $M = \sup_{[0,T] \times [0,X]} \frac{u}{H(c)}$. Under the assumption $c_- < c_+$, there exists $t_1 > t_0$, there exists $\delta > 0$ such that the solution is unique on $\mathcal{D} = \{(t, x);\ t_0 < t < t_1,\ x_0 - \delta + M(t - t_0) < x < x_0 + \delta - M(t - t_0)\}$ and presents an unique admissible shock curve issuing from (t_0, x_0).*

Proof. Let be $\delta > 0$ such that x_0 is the only discontinuity point for $c(t, x)$ in $\{0\} \times]x_0 - \delta, x_0 + \delta[$, and $X_\pm$ defined as in the proof of Lemma 6.5 (notice that $X_+ < X_-$). Let $t_1 > t_0$ be such that the solution of the ODE

$$\frac{dX}{ds}(s, t_0, x) = \alpha(s) F'\big(c\big(s, X(s, t_0, x)\big)\big), \qquad X(t_0, t_0, x) = x \tag{52}$$

exists and is unique on $]t_0, t_1[$ for $x \in]x_0 - \delta, x_0 + \delta[\setminus\{0\}$. Moreover, we can assume that

$$\sup\{c(t_0, x);\ x_0 - \delta < x < x_0\} < \inf\{c(t_0, x);\ x_0 < x < x_0 + \delta\} \tag{53}$$

and that $t_1 - t_0$ is small enough to ensure that the characteristic lines issuing respectively from $\{0\} \times]x_0 - \delta, x_0[$ and $\{0\} \times]x_0, x_0 + \delta[$ meet each other before time t_1. This last point is easily justified using (21), (53), $\inf_{[0,T]} u_b(t) > 0$ and that F' is continuous and strictly decreasing. It follows that the solution cannot be smooth in $Z = \{(s, \xi);\ t_0 < s < t_1,\ X_+(s) < \xi < X_-(s)\}$. Using the characteristic lines given by (52), we define the $\mathcal{C}^1$ functions C_- and C_+ respectively on the open sets $\mathcal{D}_- = \{(s, \xi);\ t_0 < s < t_1,\ x_0 - \delta + M(s - t_0) < x < X_-(s)\}$ and $\mathcal{D}_+ = \{(s, \xi);\ t_0 < s < t_1,\ X_+ < x < x_0 + \delta - M(s - t_0)\}$ which both contains Z. Thanks to (16), we associate them two $\mathcal{C}^1$ functions U_- and U_+. Then the ODE

$$\frac{d\xi}{ds} = \mathcal{F}\big(C_-\big(s, \xi(s)\big), C_+\big(s, \xi(s)\big)\big), \quad \xi(t_0) = x_0,$$

where $\mathcal{F}(C_-, C_+) = \frac{U_+ - U_-}{h(C_+) - h(C_-)}$ is $\mathcal{C}^1$, admits locally (on $]t_0, t_1[$, restricting t_1 if necessary) an unique solution which determines the shock curve. The entropic solution is uniquely defined for $(s, \xi) \in \mathcal{D}$, $x < \xi(s)$ or $x > \xi(s)$ by C_- or C_+, respectively.   □

Remark 6.1. If (t_0, x_0) is a point of discontinuity for u but not for c, the entropy condition (EC) implies that there is no shock curve passing through this point. The characteristic lines, locally defined around (t_0, x_0) by $\frac{dX}{ds} = \frac{[u]}{[H(c)]}$ are piecewise $\mathcal{C}^1$ and we get the local uniqueness of the solution for $t > t_0$.

Corollary 6.1. *There exists $\tau > 0$ such that the solution is unique on $(0, \tau) \times (0, X)$.*

Proof. It follows from Lemmas 6.5 and 6.6 that for all $x_0 \in (0, X)$ there exists $\delta > 0$, there exists $\tau > 0$ such that the solution is unique on $(0, \tau) \times (x_0 - \delta, x_0 + \delta)$. Then we conclude using a mere compact argument.   □

Proof of Theorem 6.1. Let

$$T^* = \sup\{\tau \in [0, T];\ \text{the solution is unique on } (0, \tau) \times (0, X)\}$$

and assume that $T^* < T$. The solution is unique on $(0, T^*) \times (0, X)$. By Corollary 6.1 there exists $\tau > 0$ such that we have uniqueness on $(T^*, T^* + \tau) \times (0, X)$. Then we have uniqueness on $(0, T^* + \tau) \times (0, X)$, contradicting the assumption. Finally $T^* = T$ and Theorem 6.1 holds.   □

Remark 6.2. In Section 2 we showed that, in the case of smooth solutions, c is the solution of the scalar conservation law (12). Thus, it is a natural question to wonder if the weak entropic solutions of (12) (in the usual sense) are the same as those of the system (8)–(9) with the entropy condition (EC) (at least in the case of uniqueness). Actually the answer is positive if and only if the function h is linear and increasing, i.e., if and only if the isotherm function is linear ($q^*(c_1, c_2) = ac_1$ with $a > 0$ or equivalently $h(c) = ac - a$). Let us briefly justify this claim. For a shock wave connecting (c_-, u_-) and (c_+, u_+), let be σ the speed of the shock given by the Rankine–Hugoniot condition for (12): $\sigma = \alpha(t) \frac{[F(c)]}{[c]}$ and let be s the corresponding speed for (8)–(9), given by (31). Writing $\alpha(t) = u_- e^{g(c_-)}$, we get

$$s = \sigma \quad \Longleftrightarrow \quad \frac{c_+ - c_-}{c_+ - c_- + c_+(h(c_+) - h(c_-))} = \frac{c_+ e^{-(g(c_+ - g(c_-)))} - c_-}{c_+ - c_-}.$$

Setting $c_- = 0$, $c_+ = x$ and using (15) we get, after differentiation with respect to x: $g(x) = \ln(1 + xh'(x))$. Differentiating again, we get finally $h'' = 0$ as a necessary condition. It is very easily shown that this condition is also sufficient. Finally if $h(c) = ac + b$ we have $g'(c) = \frac{a}{ac+1}$ and, up to an additive constant, $F(c) = \frac{c}{ac+1}$: the (EC) condition (c increases through a shock) coincides with the Oleinik condition if and only if F is concave, i.e., $a > 0$.

7. Figures

The following results have been obtained with a Langmuir isotherm, using the Godunov scheme presented in Section 4. The values of the various parameters, adapted from those in [16] are not important: our purpose is to illustrate the phenomena pointed out along the previous study. The bed profiles in the cases of adsorption or desorption steps (Figs. 2 and 3) for the Langmuir or the linear isotherm are the same as in [16], but, as pointed out in the introduction, the case of the so-called BET isotherm is out of our reach under the assumptions (10)–(11).
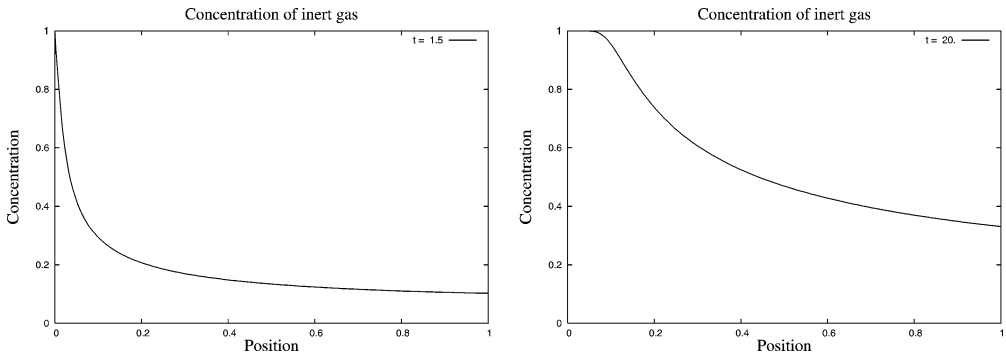

Fig. 2. Desorption step. The initial concentration is $c_0 = 0.1$, the boundary data are $c_b = 1.0$ and $u_b = 0.4$. The discontinuity at $(t = 0, x = 0)$ gives a rarefaction wave which evolves towards the steady state $c \equiv 1.0$.
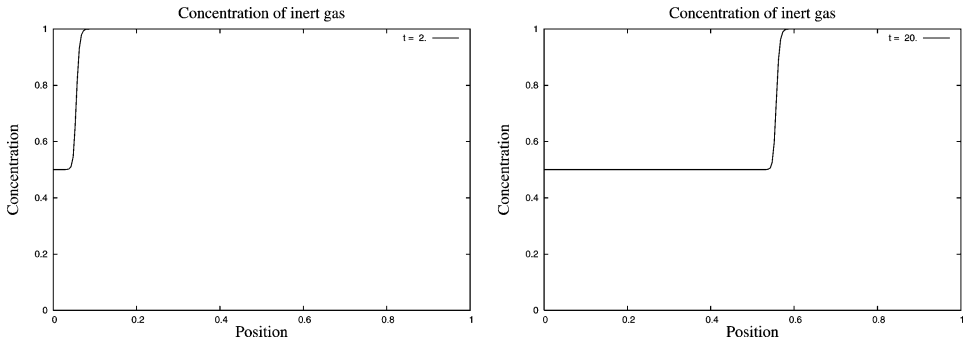

Fig. 3. Adsorption step. The initial concentration is $c_0 = 1.0$, the boundary data are $c_b = 0.5$ and $u_b = 2.0$. The discontinuity at $(t = 0, x = 0)$ gives a shock wave which propagates to the right. The concentration c of the inert gas evolves towards the steady state $c \equiv 0.5$.
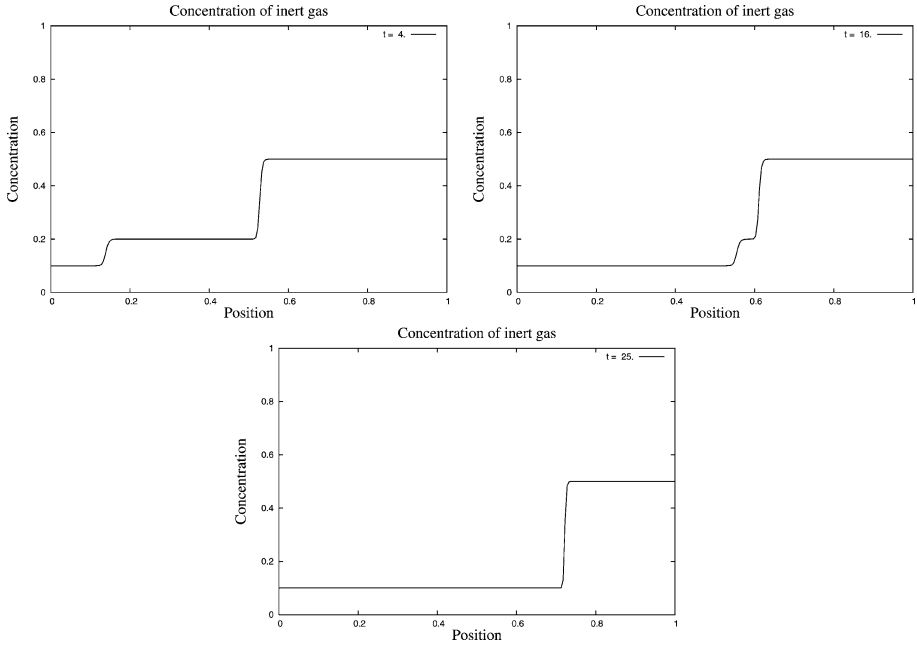
Fig. 4. Double shock. The initial concentration is $c_0 = 0.2$ for $x \leqslant 0.5$ and $c_0 = 0.5$ for $x > 0.5$, the boundary data are $c_b = 0.1$ and $u_b = 0.5$. Both discontinuities at $(t = 0, x = 0)$ and $(t = 0, x = 0.5)$ give a shock wave which propagates to the right. The "small shock" catches the other and merge into a single one. The concentration c of the inert gas evolves towards the steady state $c \equiv 0.1$.
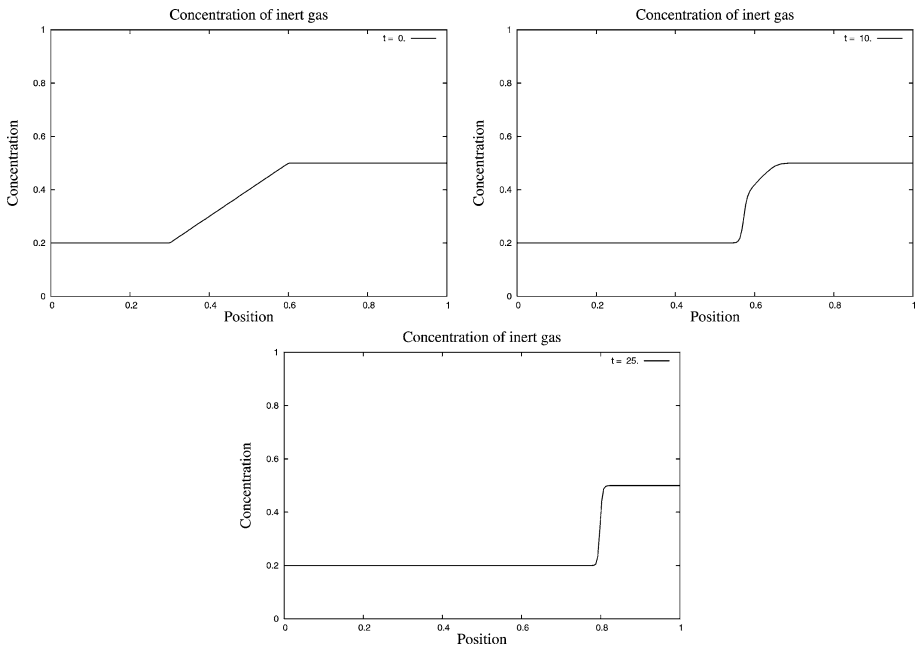

Fig. 5. Development of a shock. The initial concentration is continuous and increasing, there is no discontinuity at $(t = 0, x = 0)$. Boundary data are $c_b = 0.2$ and $u_b = 0.5$.

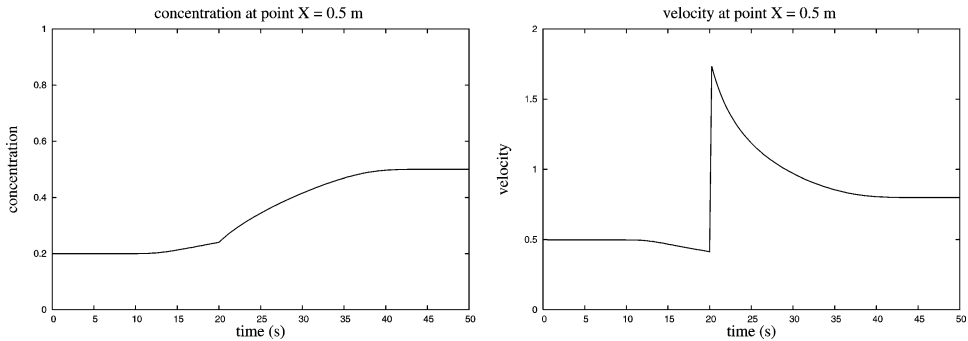Fig. 6. Contact discontinuity. We start with a rarefaction wave arising from a discontinuity at ($t = 0$, $x = 0$) with $c_0 = 0.2$ and $c_b = 0.5$. The velocity u_b is 0.2 for $t \leqslant 20$ and 0.8 for $t > 20$. c remains continuous while the discontinuity of the velocity u "propagates at infinite speed." We show the evolution of c and u at the position $x = 0.5$. Notice that the maximum principle is not valid for u.

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