Eulerian and Lagrangian formulations in BV^s for gas-solid chromatography

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ABSTRACT. –An initial-boundary value problem for a chemical system with unknown velocity related to gas chromatography is considered. The system is hyperbolic and existence of entropy solutions is achieved in fractional BV spaces: BV^s, $s \geq 1/3$, with less regularity than usual. We prove that $BV^{1/3}$ is the critical space for this problem. A Lagrangian formulation of the system for the initial value problem provides a smoothing effect in BV and uniqueness when the first gas is more active than the second one.

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Key words: chromatography; conservation laws; fractional BV spaces; boundary problem; convex flux; entropy solution; Lagrangian coordinates; Cauchy problem; uniqueness; regularity.

Contents

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Introduction

A chemical model of fixed-bed adsorption of gases is widely used in chemical engineering ([21]). This model is known to be a hyperbolic system of PDEs [26, 27]. Up to our knowledge, the first study of the Riemann Problem for two species was done by chemists in [16]. The first mathematical study was done in BV framework in [4] for an inert gas and a convex isotherm. Fractional BV spaces, the so called BV^s, $0 < s < 1$, naturally appear for conservation laws ([9] completed and generalized in [13]). The first aim of this paper is to obtain the existence of entropy solutions for a 2×2 gas-solid chromatography system in the spaces BV^s, $s \geq 1/3$. It was shown in a previous work ([8]) that only for L^∞ data blow up can occur and in some sense this existence in the critical space $BV^{1/3}$ is optimal. This result was announced in [10]. The second aim of this paper is to write this 2×2 gas chromatography system in Lagrangian coordinates. The new system for the Cauchy problem provides a smoothing effect for the concentration in BV as in [18, 20] and also uniqueness for concave isotherms (Langmuir).

The article is organized as follows. Section 1 presents the derivation of the dimensionless chemical model to yield an initial-boundary value problem. Section 2 deals with the existence of the initial-boundary value problem in BV^s for $s \geq 1/3$. The Euler-Lagrange change of variables and the Lagrangian formulation are performed in Section 3. Finally, a smoothing effect and the uniqueness of entropy solutions for the Cauchy problem through the Lagrangian formulation are given in the last section.

1 The Chemical model: a hyperbolic system

1.1 The dimensionless model

"Pressure Swing Adsorption (PSA) is a technology that is used to separate some species from a gas under pressure according to these species' molecular characteristics and affinity for an adsorbent material. It operates at near-ambient temperatures and so differs from cryogenic distillation techniques of gas separation. Special adsorptive materials (e.g., zeolites) are used as a molecular sieve, preferentially adsorbing the undesired gases at high pressure. The process then swings to low pressure to desorb the adsorbent material. Using two adsorbent vessels allows near-continuous production of the target gas. It also permits the so-called pressure equalization, where the gas leaving the vessel being depressurized

is used to partially pressurize the second vessel. This results in significant energy savings, and is common industrial practice." (Wikipedia)

PSA is used extensively in the production and purification of oxygen, nitrogen and hydrogen for industrial uses. It can also be used to separate a single gas from a mixture of gases. A typical PSA system involves a cyclic process where a number of connected vessels containing adsorbent material undergo successive pressurization and depressurization steps in order to produce a continuous stream of purified product gas.

We focus on a model describing a step of the cyclic process, restricted to isothermal behavior. As in general fixed bed chromatography, each of the d species ($d \geq 2$) simultaneously exists under two phases, a gaseous and movable one with concentration $c_i(t,x)$ or a solid (adsorbed) other with concentration $q_i(t,x)$, $1 \leq i \leq d$. In gas chromatography, velocity variations accompany changes in gas composition, especially in the case of high concentration solute: it is known as the sorption effect. This effect is taken into account through a constraint on the pressure. The reader can refer for instance to [16] :"Fixed-Bed Adsorption of Gases : Effect of Velocity Variations on Transition Types".

In this section we show how to obtain, under some assumptions, the dimensionless model which is the subject of our study (see also [4, 5, 7, 8]). The original model, nothing else that material balances for two adsorbable components, writes:

$$\begin{aligned} \rho_b\, \partial_t q_i + \partial_t(\varepsilon\, c_i) + \partial_z(u\, c_i) &= 0, \quad i \in \{1,2\}, && (1)\\ c_1 + c_2 &= c, && (2) \end{aligned}$$

where

$c_i\,(moles/m^3)$, $i \in \{1,\,2\}$, is a fluid-phase concentration and $q_i\,(moles/kg)$, $i \in \{1,\,2\}$, is the corresponding adsorbed-phase concentration,

$u\,(m/s)$ is the superficial fluid velocity (the same for the two components),

$c\,(moles/m^3)$ in (2) is a constant because temperature and pressure are assumed to be constant: this constraint is related to the sorption effect, as explained before,

ε is the local fraction of the bed occupied by gas, including that within the pore space of the absorbent. It is assumed to be constant, which means that the local fraction of the bed occupied by gas is not affected by the adsorbed components,

$\rho_b\,(kg/m^3)$ is the bulk density of packing.

Notice that the so-called isotherms $q_i = q_i(c_1, c_2)$ satisfy

$$\frac{\partial q_i}{\partial c_i} \geq 0, \quad i \in \{1,2\}. \tag{3}$$

In [16] it is assumed that the incoming velocity of the mixture is a constant $u_b > 0$ but in the sequel we will only assume that there exists $u_0 > 0$ such that $u_b(t) \geq u_0 > 0$ and we set $u^* = u/u_0$.

Using the change of variables $\tau = t/T$, $x = \varepsilon z/u_0 T$, where T is a characteristic duration of a pressurization or depressurization step, we can write (1-2) under the dimensionless form:

$$\begin{aligned} \partial_\tau(\tilde{c_i} + q_i^*(\tilde{c_1}, \tilde{c_2})) + \partial_x(u^*\,\tilde{c_i}) &= 0, \quad i \in \{1,2\}, & (4)\\ \tilde{c_1} + \tilde{c_2} &= 1, & (5) \end{aligned}$$

where we have set

$$\tilde{c_i} = c_i/c, \quad q_i^* = \rho_b\, q_i/\varepsilon c.$$

Changing the notations, we write this system under the form:

$$\begin{aligned} \partial_t(c_1 + q_1^*(c_1, c_2)) + \partial_x(c_1\, u) &= 0, & (6)\\ \partial_t(c_2 + q_2^*(c_1, c_2)) + \partial_x(c_2\, u) &= 0, & (7)\\ c_1 + c_2 &= 1. & (8) \end{aligned}$$

Next, we set $c = c_1 \in [0,1]$ (then $c_2 = 1 - c$), $q_i(c) = q_i^*(c, 1-c)$, $i = 1, 2$ and we obtain finally the following system which is the object of our study for $x > 0$ and $t > 0$:

$$\begin{aligned} \partial_x(c\, u) + \partial_t I(c) &= 0, & (9)\\ \partial_x u + \partial_t h(c) &= 0, & (10) \end{aligned}$$

where

$$h(c) = q_1(c) + q_2(c) \geq 0, \quad I(c) = c + q_1(c).$$

Following [16], we introduce a key function which will play a central role in the nonlinear study of the system, namely,

$$f = c_2\, q_1 - c_1\, q_2 = q_1(c) - c\, h(c). \tag{11}$$

Throughout this paper we assume

$$f''(c) \neq 0 \text{ and } h'(c) > -1 \text{ for all } c \in [0,1], \tag{12}$$

which is relevant for a large class of isotherms exchanging c_1 and c_2 if necessary ([7]). With theses notations, the relations (3) read $q_1' \geq 0 \geq q_2'$.
We will also make use of following functions only depending on the isotherms [5]:

- $H(c) = 1 + q_1' - ch' = 1 + (1-c)q_1' - cq_2' \geq 1$,
- $G(c) = \exp g(c)$ where $g' = -\dfrac{h'}{H}$.

1.2 The hyperbolic initial-boundary value problem

It is possible to analyze system (9)-(10) in terms of hyperbolic system of PDEs provided we exchange the time and space variables (cf [5]). The initial-boundary value problem

is then system (9)-(10) for $x > 0$ and $t > 0$ supplemented by the initial ($x = 0$) and boundary data ($t = 0$):

$$\begin{cases} c(0,t) = c_b(t), & t > 0, \\ u(0,t) = u_b(t), & t > 0, \\ \\ c(x,0) = c_0(x), & x \in \mathbb{R}_+, \end{cases} \tag{13}$$

where

$$0 \leq c_b, c_0 \leq 1, \tag{14}$$

$$0 < \inf_{\mathbb{R}} u_b \leq \sup_{\mathbb{R}} u_b < +\infty. \tag{15}$$

For this system, the surprising point is the first two equations of (13) correspond to the initial data and the last one to the boundary data. That is to say that the variable x is progressive: time-like and t is a space-like variable. To be clear, we distinguish the physical time t to the mathematical time or hyperbolic time x.

We also study in Lagrangian variables the mathematical initial value problem which is system (9), (10) for $x > 0$ and $t \in \mathbb{R}$ (notice that t negative is considered) supplemented with initial data:

$$\begin{cases} c(0,t) = c_b(t), & t \in \mathbb{R}, \\ u(0,t) = u_b(t), & t \in \mathbb{R}. \end{cases} \tag{16}$$

The mathematical initial value problem is physically relevant for applications because experimenters only control c_b, u_b, and c_0 can be viewed as an equilibrium reached before the beginning of the process. Moreover, the information propagates with a finite speed and we only need to know u_b, c_b on a compact set.

We have shown in [5] that there are two families of entropies: $u\,\psi(c)$ and $\phi(u\,G(c))$, where ϕ and ψ are any real smooth functions. The corresponding entropy flux $Q(c)$ of the first family satisfies

$$Q'(c) \;\; = \;\; h'(c)\,\psi(c) + H(c)\,\psi'(c).$$

The first family is degenerate convex (in variables (u, uc)) provided $\psi'' \geq 0$. So we seek entropy solutions which satisfy

$$\partial_x\,(u\,\psi(c)) + \partial_t Q(c) \leq 0,$$

in the distribution sense. The second family is not always convex. There are only two interesting cases where this family is convex, namely $\pm G''(c) > 0$ for all $c \in [0,1]$. When $G'' > 0$ and $\alpha > 1$, we expect to have $\partial_x (u\,G(c))^\alpha \leq 0$ which reduces to $\partial_x (u\,G(c)) \leq 0$. In the same way, if $G'' < 0$, we get $\partial_x (u\,G(c)) \geq 0$.

Now we recall a mathematical definition of entropy solutions.

Definition 1.1 *Let $T > 0$, $X > 0$, $u \in L^\infty((0,T) \times (0,X), \mathbb{R}^+)$, $0 \leq c(t,x) \leq \rho \equiv 1$ for almost all $(t,x) \in (0,T) \times (0,X)$. Then (c,u) is an* **entropy solution** *of system (9)-(10) with respect to the family of entropies $u\,\psi(c)$ if, for all convex function (or degenerate convex) ψ,*

$$\frac{\partial}{\partial x}\,(u\,\psi(c)) + \frac{\partial}{\partial t} Q(c) \;\; \leq \;\; 0, \tag{17}$$

in $\mathcal{D}'([0,T)\times[0,X))$, *where* $Q'=H\psi'+h'\psi$, *that is, for all* $\phi\in\mathcal{D}([0,T)\times[0,X);\mathbb{R}_+)$,

$$\int_0^X\int_0^T \left(u\,\psi(c)\,\partial_x\phi+Q(c)\,\partial_t\phi\right)\,dt\,dx+\int_0^T u_b(t)\,\psi(c_b(t))\,\phi(t,0)\,dt + \int_0^X Q(c_0(x))\,\phi(0,x)\,dx\geq 0.$$

For this system we reformulate the global existence theorem of entropy solutions with BV concentration (cf [5]) .

Theorem 1.1 (Existence in BV) *Assume* (12) *on isotherms,* $c_0\in BV([0,+\infty)_x,[0,1])$, $c_b\in BV([0,+\infty)_t,[0,1])$ *and* $\ln u_b\in L^\infty([0,+\infty)_t,\mathbb{R})$, *then the initial-boundary value problem* (9), (10) *on* $[0,+\infty)_x\times\mathbb{R}_t$ *with initial-boundary data* c_b, u_b, c_0 *in* (13) *admits a global weak entropy solution* (c,u). *Furthermore, we have the following estimates:*

$$\begin{aligned} &0\leq c\leq 1,\\ c\in L^\infty([0,+\infty)_x;BV([0,+\infty)_t))\quad &\cap\quad L^\infty([0,+\infty)_t;BV([0,+\infty)_x)),\\ \ln u\in L^\infty([0,+\infty)_t;BV([0,+\infty)_x)).&\end{aligned}$$

The proof of Theorem 1.1 uses a adapted Godunov scheme given in [4, 5]. The assumption (12) is useful to ensure the hyperbolicity of the PDE system (9), (10). This assumption is not needed when only one gas is active and the other is inert ([4]). For two active gases, condition (12) is discussed in section 2.1 for the Riemann Problem.

A goal of this article is to state an existence result in a more general functional context of fractional BV spaces BV^s which appears to be the critical spaces for the existence or not of entropy solutions for this system.

2 Existence with BV^s concentrations

In this section, we give the main result and its proof. The existence is given by a Godunov scheme and estimates about c and $\ln u$ using BV^s spaces. Spaces $BV^s(I)$, for $0<s\leq 1$ appear to be a generalization of $BV(I)$, spaces of functions with a bounded variation on I (I is a non empty interval of $\mathbb{R}$). They are defined as follows.

Definition 2.1 (Definition of $BV^s(I)$) *We denote by* $\mathcal{S}(I)$ *the set of the subdivisions of* I, *that is the set of finite subsets* $\sigma=\{x_0,x_1,\cdots,x_n\}\subset I$ *with* $x_0<x_1<\cdots<x_n$.

Let $\sigma=\{x_0,x_1,\cdots,x_n\}\in\mathcal{S}(I)$ *and let* u *be a real function defined on* I. *The* s*-total variation of* u *with respect to* σ *is*

$$TV^s u\{\sigma\} \;=\; \sum_{i=1}^{n}|u(x_i)-u(x_{i-1})|^{1/s} \tag{18}$$

and the s*-total variation of* $u(.)$ *on* I *is defined by*

$$TV^s u\{I\}=\sup_{\sigma\in\mathcal{S}(I)} TV^s u\{\sigma\}, \tag{19}$$

where the supremum is taken over all the subdivisions σ of I. The set $BV^s(I)$ is composed of functions $u : I \to \mathbb{R}$ such that $TV^s u\{I\} < +\infty$. We define the BV^s semi-norm by

$$|u|_{BV^s(I)} = (TV^s u\{I\})^s . \tag{20}$$

If $0 < s < t \leq 1$ and I is not reduced to one point then $BV^t(I) \subsetneq BV^s(I)$. The following inclusion is obtained directly from the definition. For an interval I of $\mathbb{R}$,

$$\forall s \in (0,1], \quad BV^s(I) \subset L^\infty(I).$$

Notice that $\bigcup_{s>0} BV^s$ is strictly smaller than L^∞ since bigger generalized BV spaces called BV_Φ belong also in L^∞ ([13]).

We also recall the following elementary lemma which is quite different from the case $s = 1$.

Lemma 2.1 *If $0 < s < 1$ and $(a_i)_{1\leq i\leq n}$ is a finite sequence of positive real numbers, then*

$$\sum_{1\leq i\leq n} a_i^{1/s} < \left(\sum_{1\leq i\leq n} a_i\right)^{1/s} .$$

This inequality is the converse of the usual triangular inequality. This is the reason why BV^s estimates require to consider all subdivisions (not only the finest ones) unlike the BV framework. Nevertheless, spaces BV^s are well fitted for sharp estimates in the context of scalar conservation laws (cf [9, 12]) and used now for the 2×2 adsorption system.

Theorem 2.1 (Existence in BV^s for $s \geq \frac{1}{3}$)
Let $\frac{1}{3} \leq s \leq 1$, $X > 0$, $T > 0$. If $c_b \in BV^s([0,T],[0,1])$, $c_0 \in BV^s([0,X],[0,1])$, $\ln u_b \in L^\infty([0,T],\mathbb{R})$ and condition (12) on isotherms is fulfilled, then there exists an entropy solution (c,u) on $[0,X]\times[0,T]$ of the initial-boundary value problem (9)-(10)-(13) such that

$$\begin{gathered} 0 \leq c \leq 1, \\ c \in L^\infty([0,T], BV^s([0,X])), \\ \ln u \in L^\infty([0,T]\times[0,X]). \end{gathered}$$

It turns out that if c_0, c_b belong to $BV^{1/3}$ then there is no blow up of the velocity at the characteristic boundary and if the initial concentration c_0 does not belong to $BV^{1/3}$ the blow-up can occur as suggested in [10]. If $s < 1/3$ a blow-up is exhibited in Section 2.3, hence we need $c \in BV^s_x$ with $s \geq 1/3$ in the previous result.

2.1 Riemann Problem for the Eulerian system

To be self-contained, the solution of the Riemann problem is briefly expounded, more details are in [5, 7, 8] (notice that the notations are not uniform in the previous papers). The PSA system admits two eigenvalues: 0 and $\lambda = \dfrac{H(c)}{u} > 0$ ([5]). It is more convenient to begin by the resolution of the boundary Riemann problem which is characteristic. The complete Riemann problem is solved at the end of this subsection with the hyperbolic time x and then with the physical time t.

The boundary Riemann problem has the form:

$$\begin{cases} \partial_x u + \partial_t h(c) &= 0, \\ \partial_x(uc) + \partial_t I(c) &= 0, \end{cases} \tag{21}$$

$$c(0,x) = c^0 \in [0,1], \quad x > 0, \qquad \begin{cases} c(t,0) &= c^+ \in [0,1], \\ u(t,0) &= u^+ > 0, \end{cases} \quad t > 0. \tag{22}$$

We are looking for a self-similar solution, i.e.,

$$c(t,x) = C(z), \quad u(t,x) = U(z) \text{ with } z = \frac{t}{x} > 0.$$

In the domain $t > 0, x > 0$, the boundary Riemann problem is solved with a $\lambda-$rarefaction wave or a $\lambda-$shock wave since λ is the only positive eigenvalue of the system and λ is genuinely nonlinear from convex assumption (12).

Proposition 2.1 (([5]) $\lambda-$rarefaction waves)
Any smooth non-constant self-similar solution $(C(z), U(z))$ of (21) in an open domain $\Omega = \{0 \le \alpha < z < \beta\}$ where $f''(C(z))$ does not vanish, satisfies

$$\frac{dC}{dz} = \frac{H(C)}{z\, f''(C)}, \quad U(z) = \frac{H(C)}{z}.$$

In particular, $\dfrac{dC}{dz}$ has the same sign as $f''(C)$.

Assume for instance that $0 \le a < c^0 < c^+ < b \le 1$ and $f'' > 0$ in (a,b). Then the only smooth self-similar solution of (21) is such that

$$\begin{cases} C(z) &= c^0, & 0 < z < z_0, \\ \dfrac{dC}{dz} &= \dfrac{H(C)}{z\, f''(C)}, & z_0 < z < z_+, \\ C(z) &= c_+, & z_+ < z, \end{cases} \tag{23}$$

where

$$z^+ = \frac{H(c^+)}{u^+}, \quad z^0 = z^+ e^{-\Phi(c^+)} \text{ with } \Phi(c) = \int_{c^0}^{c} \frac{f''(\xi)}{H(\xi)}\, d\xi.$$

Moreover, $u^0 = \dfrac{H(c^0)}{z^0}$ and U is given by

$$\begin{cases} U(z) &= u_0, & 0 < z < z_0, \\ U(z) &= \dfrac{H(C(z))}{z}, & z_0 < z < z_+, \\ U(z) &= u_+ & z_+ < z. \end{cases} \tag{24}$$

Proposition 2.2 (([5]) $\lambda-$shock waves) *If (c^0, c^+) satisfies the following admissibility condition equivalent to the Liu entropy-condition:*

$$\text{for all } c \text{ between } c^0 \text{ and } c^+, \quad \frac{f(c^+) - f(c^0)}{c^+ - c^0} \leq \frac{f(c) - f(c^0)}{c - c^0},$$

then the Riemann problem (21) is solved by a shock wave defined as

$$C(z) = \begin{cases} c^0 & \text{if} \quad 0 < z < s, \\ c^+ & \text{if} \quad s < z, \end{cases} \qquad U(z) = \begin{cases} u^0 & \text{if} \quad 0 < z < s, \\ u^+ & \text{if} \quad s < z, \end{cases} \tag{25}$$

where u^0 and the speed s of the shock are obtained through

$$u^0([I] - c^0[h]) = u^+([I] - c^+[h]), \qquad s = \frac{[h]}{[u]}, \tag{26}$$

with

$$[u] = u^+ - u^0, \quad [h] = h(c^+) - h(c^0), \quad [I] = I(c^+) - I(c^0).$$

The notation of the function h is different in [4] so the jump conditions are rewritten.

Proof of Prop.2.2: from (9), (10) the Rankine-Hugoniot conditions read with the shock speed $s = \dfrac{dt}{dx} \neq 0$, $s[u] = [h]$ and $s[uc] = [I]$. Thus $[uc][h] = [u][I]$ and also the relation (26) allows to compute u^0 and then s. □

Now, for PSA system (21), we solve the Riemann problem with the following initial data:

$$\begin{cases} c(t,0) &= c^- \in [0,1], \\ u(t,0) &= u^- > 0, \end{cases} \quad t < 0, \quad \begin{cases} c(t,0) &= c^+ \in [0,1], \\ u(t,0) &= u^+ > 0, \end{cases} \quad t > 0. \tag{27}$$

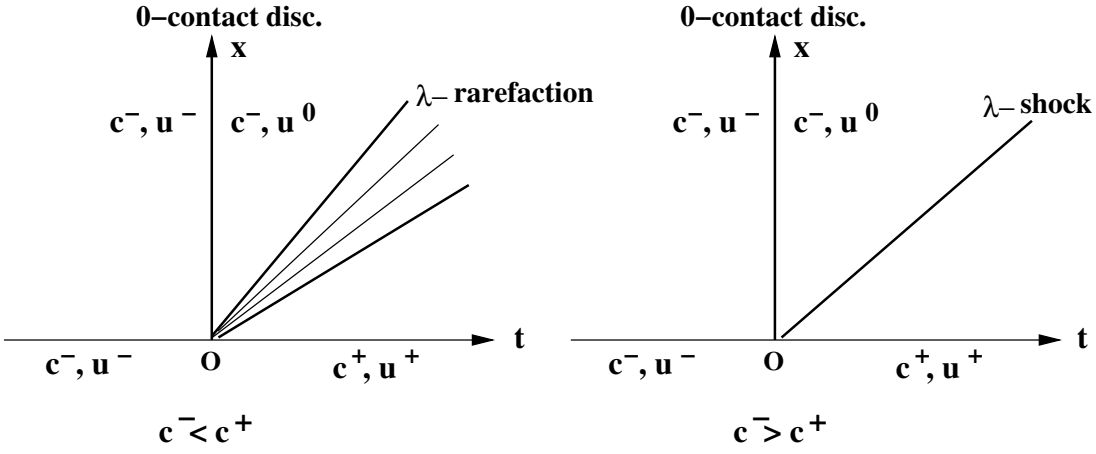

Figure 1: solution of the Riemann problem when $f'' > 0$.

A $0-$wave appears on the line $\{t = 0\}$. The solution of the Riemann problem for $x > 0$ with a convex function f is

- $(c, u) = (c^-, u^-)$ for $t < 0$,
- a $0-$contact discontinuity for $t = 0$,
- a $\lambda-$ wave for $t > 0$,

see Fig. 1. In practice, since $c^0 = c^-$, we first solve the boundary Riemann Problem (21), (22). Then u^0 is well defined and the $0-$contact discontinuity is automatically solved.

To obtain global BV estimates on the concentration, it was shown in [4, 5] that the physical time t yields to simpler estimate than with the hyperbolic time x. Moreover, the corresponding Glimm functional is linear (as for the isothermal gas dynamic) with the physical time t and this functional is still quadratic with the hyperbolic time x ([7]). This is a reason why, we use the following physical Riemann problem with the physical time and not the hyperbolic time, see Fig. 2. As for the previous Riemann problem, the initial data are piecewise constant but now are given on the x axis:

$$\left\{\begin{array}{rcl} c(0,x) & = & c^- \in [0,1], \\ u(0,x) & = & u^- > 0, \end{array}\right. \quad x < 0, \qquad \left\{\begin{array}{rcl} c(0,x) & = & c^+ \in [0,1], \\ u(0,x) & = & u^+ > 0, \end{array}\right. \quad x > 0. \tag{28}$$

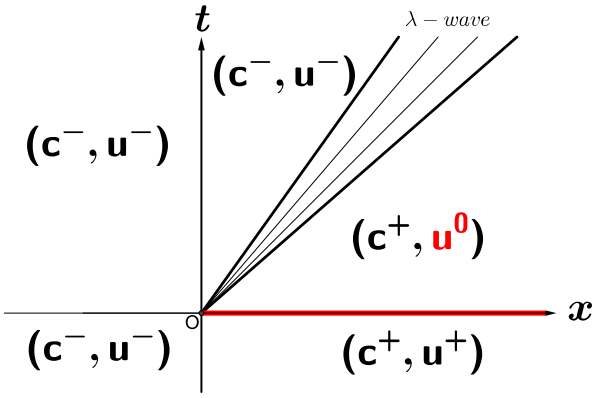

Figure 2: Physical Riemann problem

There is a λ-wave, which is a rarefaction wave or a shock wave when f is convex (or concave). The difference with a classic Riemann problem is the jump for the velocity at $t = 0$, $x > 0$: $u = u^+$ for $t < 0$ and $u = u^0$ for $\lambda\, x > t > 0$ (under the λ-wave). There is never a discontinuity on a horizontal line for a classic Riemann problem, nevertheless, the problem is tractable. Notice also that the initial value Riemann problem and the initial-boundary value Riemann problem have the same solution in $x > 0, t > 0$. Now, a key point to keep the hyperbolicity of system (9)-(10) is to keep u positive. In all previous works of the authors ([4, 5, 7, 8]) this assumption is made. Here we show that under suitable assumptions we get $u > 0$ after solving the Riemann problem.

Proposition 2.3 ($u > 0$ **for the Riemann problem)** *If convex assumption* (12) *is fulfilled and*

$$-1 < \inf_{[0,1]} h'(c) \qquad or \qquad \sup_{[0,1]} h'(c) < 1 \tag{29}$$

then the solution of the Riemann problem involves a positive velocity.

If $h' > 0$ (or $h' < 0$) then condition (29) is fulfilled. This is an important chemical case which means that one gas is more active than the other one, for examples,

- one inert gas and one active gas ([4]),
  (For the inert gas $c = c_1$ then $q_1 = 0$ and $h' = q_1' + q_2' = q_2' < 0 < 1$).
- two active gases with the binary Langmuir isotherms ([7] Proposition 5.1).

Proof: notice that if the labels for the first and the second gases are exchanged, this means that the function $h(c)$ is replaced by the function $h(1-c)$ and the condition $-1 < h'$ also reads $h' < 1$.

This result is the same for the Cauchy problem or the boundary problem as illustrated in Fig. 2, so we consider the boundary value problem (21), (22). Since f is convex or concave, u is monotonic along a λ-wave according to (24) ([5]) so we only need to prove that $u_0 > 0$. A λ-wave is a rarefaction wave or a shock wave. First, for a rarefaction wave the Riemann invariant $W = uG(c)$ is constant along this wave, so $u^- G(c^-) = u^0 G(c^+)$, and since $G > 0$, we obtain $u_0 > 0$. Second, for a shock wave, denoted by $[c] = c^+ - c^0 \neq 0$, equation (26) is rewritten as

$$u^0 \left(\frac{[I]}{[c]} - c^0 \frac{[h]}{[c]} \right) = u^+ \left(\frac{[I]}{[c]} - c^+ \frac{[h]}{[c]} \right).$$

Recall that $I(c) = c + q_1(c)$ with $q_1' \geq 0$ so $I' \geq 1$ and $\dfrac{[I]}{[c]} - c^0 \dfrac{[h]}{[c]} \geq 1 - \sup h' > 0$ since $h'(c) < 1$ on $[0, 1]$. The other term with c^+ is also positive so $u^0 > 0$. □

2.2 Proof of Theorem 2.1: existence for $s \geq \dfrac{1}{3}$

In order to get a general existence result via the construction of a sequence of approximate solutions, we are going to use, as in [4, 5], the modified Godunov scheme to system (9)-(10) in the BV^s framework ([9]): the first step is the resolution of the Riemann problem. The key point to get the BV^s estimates is the suitable choice between the "physical variables" with t as evolution variable or the "hyperbolic variables" with x as a time variable. Moreover, BV^s estimates are more difficult to handle than BV ones (as pointed out in [9]). However, we were led to favor the first approach -t as evolution variable- as in [4] than the other, in [7], which appears to be more complicated. That is why we use the Eulerian formulation.

The corresponding (CFL) condition requires a upper bound for u which is obtained thanks to the L^∞ control of $\ln u$ and we get a BV^s bound for the concentration c.

Notice also that the BV^s estimate for the concentration c is straightforward in Lagrangian variables thanks to [9] because c is the entropy solution of the scalar conservation law (38), but the advection equation (39) does not provide any L^∞ estimates for $\ln v = -\ln u$ because $h(c)$ is not regular enough (Lipschitz). It is another reason why we use Eulerian coordinates instead of Lagrangian coordinates in this section. Moreover, we show how to recover the BV^s estimate for c in this framework.

The Godunov scheme in Eulerian variables is based on the resolution of the Riemann problem in space-time boxes $B_{i,j} = [x_i, x_{i+1}) \times [t_j, t_{j+1})$ according to Fig. 3 ([4]), using the "physical variables". Here, the contact discontinuity associated to the 0-wave (in hyperbolic variables) is horizontal in physical variables and only affects u. The shock or rarefaction wave is associated to the λ-wave with speed $\dfrac{dx}{dt} = \dfrac{u}{H(c)} < u$. In Fig. 3, we have $z_\pm = u_\pm / H(c_\pm)$ for rarefaction, and $s > 0$ for shock.

As in the Lagrangian framework, the essential fact is that c is monotone in each box. Let $T > 0$, $X > 0$ be fixed. For a fixed integer N we set

$$\Delta x = \frac{X}{N+1} \quad \text{and} \quad \Delta t = \frac{T}{M+1},$$

where M is an integer depending upon N and is chosen to satisfy a CFL-type condition which writes here

$$\sup_{[0,\Delta t[\times[0,\Delta x[} u = \max(u_-, u_+) < \frac{\Delta x}{\Delta t}\,. \tag{30}$$

If this CFL condition is always satisfied, we can compute an approximate solution (c^N, u^N) row by row (i.e. for each fixed $j \in \{0, \cdots, M\}$) solving the Riemann problem on each box $B_{i,j}$, $i = 0, \cdots, N$.

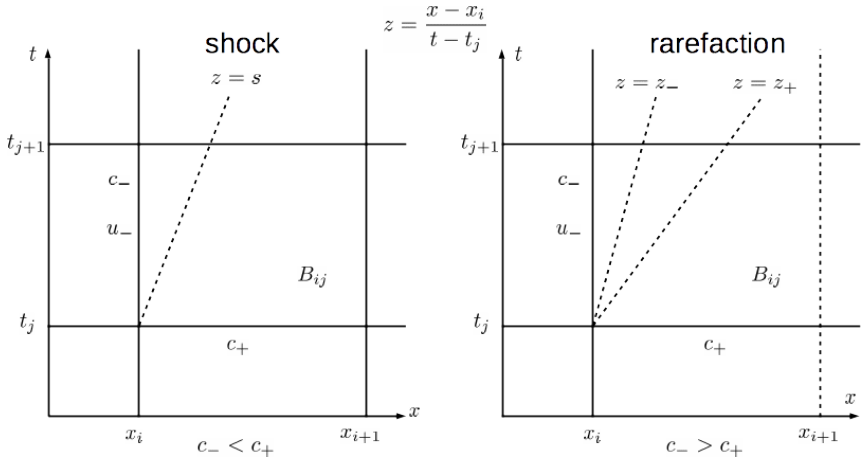

Figure 3: *the Riemann problem in a box B_{ij}, case $f'' < 0$.*

The s-total variation of the concentration is controlled by the initial-boundary s-total variation $TV^s c_{IB} = TV^s c_{IB}\{[-T, X]\}$ where c_{IB} is defined as

$$c_{IB}(y) = \begin{cases} c_b(-y) & \text{if} \quad -T \le y < 0, \\ c_0(y) & \text{if} \quad 0 \le y \le X. \end{cases}$$

Proposition 2.4 (BV^s estimate for the Godunov scheme) *Let $(c^N, u^N)_N$ be the sequence of approximate solutions constructed by the Godunov scheme in Eulerian variables. If the CFL condition (30) is fulfilled, then $TV^s c\{[0, X]\} \leq TV^s c_{IB}$.*

Proof: the general structure of the proof follows from those of [4, 5] and we only focus on the differences due to the BV^s framework instead of BV. The first step is the discretization of the initial-boundary data c_0 and c_b in order to start with a step function. This is achieved without increasing the s-total variation taking classically the mean value in each cell as proved in Lemma 2.2.

The second step consists in the resolution of the Riemann problems associated to the first row $(B_{i,0})_{0\leq i\leq N}$. For $t < t_1$, we denote $(c^N(\cdot, t), u^N(\cdot, t))$ the solution at time t and we focuse on c^N.
In the interval $]x_{i-1}, x_{i+1}[$ (notations of Fig. 3) $c^N(\cdot, t)$ is constant on $]a_i(t), a_{i,1}(t)[$ with value c_i and on $]a_{i+1}(t), x_{i+1}[$ with value c_{i+1} (see Fig. 4) where $x_{i-1} < a_{i,1}(t) \leq a_{i+1}(t) < x_{i+1}$, i.e. out of the wave fan issued from $(x_i, 0)$, and $c^N(., t) = c_{i,1}(., t)$ on $]a_{i,1}(t), a_{i+1}(t)[$. Notice that we have $a_{i,1}(t) = a_{i+1}(t)$ if and only if the wave is a shock. We set $M_i =]a_i(t), x_{i+1}[$: according to Prop. 2.1 $c^N(., t)$ is monotone on M_i.

Let $\sigma = \{\xi_0, \cdots, \xi_p\}$ be a subdivision of $[0, X]$ and

$$TV^s c^N(\cdot, t)\{\sigma\} = \sum \mid c^N(\xi_i, t) - c^N(\xi_{i-1}, t) \mid^{1/s} .$$

Let $\tilde{\sigma}$ be the subdivision obtained by removing the points ξ_i located in a "λ-wave fan", i.e.: $\tilde{\sigma} = \sigma \setminus \bigcup_n [x_i, a_{i+1}(t)]$. We are going to show that it is possible to add to $\tilde{\sigma}$ a finite set P of points located in $\bigcup_n]a_i(t), x_i[$ in such a way that

$$TV^s c^N(\cdot, t)\{\tilde{\sigma} \cup P\} \geq TV^s c^N((\cdot, t)\{\sigma\}.$$

This being carried out, we get

$$TV^s c^N(\cdot, t)\{\sigma\} \leq TV^s c^N(\cdot, t)\{\tilde{\sigma} \cup P\} \leq TV^s c_{IB}.$$

In the bounded interval $[\min \sigma, \max \sigma]$ there is a finite number of wave fans and we just need to consider the case of the one issued from $(x_i, 0)$ and its associated monotony zone M_i in which we assume (for instance) that $c^N(\cdot, t)$ is decreasing, as in Fig. 4.
If $\sigma \cap M_i = \emptyset$ then we have nothing to do, else we set $k(i) = \max\{0 \leq k \leq p\,;\, \xi_k \leq x_i\}$ (if exists) and $\ell(i) = \min\{0 \leq k \leq p\,;\, \xi_k \geq a_{i+1}(t)\}$ (if exists).

- If $k(i)$ exists and $c^N(\xi_{k(i)}, t) < c_i$ then we add to $\tilde{\sigma}$ any point $y_{k(i)} \in]a_i(t), x_i]$,
- if $\ell(i)$ exists and $c^N(\xi_{\ell(i)}, t) > c_{i+1}$ then we add to $\tilde{\sigma}$ any point $y_{\ell(i)} \in]a_{i+1}(t), x_{i+1}[$,

else we have nothing to do.
Let P be the set of the added points according to the preceding procedure. Thanks to Lemma 2.1, we get immediately

$$TV^s c^N(\cdot, t)\{\sigma^*\} \geq TV^s c^N(\cdot, t)\{\sigma\}, \quad \text{where} \quad \sigma^* = \tilde{\sigma} \cup P.$$

Moreover, $TV^s c^N(\cdot,t)\{\sigma^*\}$ is constant on $[0,t_1[$ and thus is controlled by $TV^s c_{IB}$.

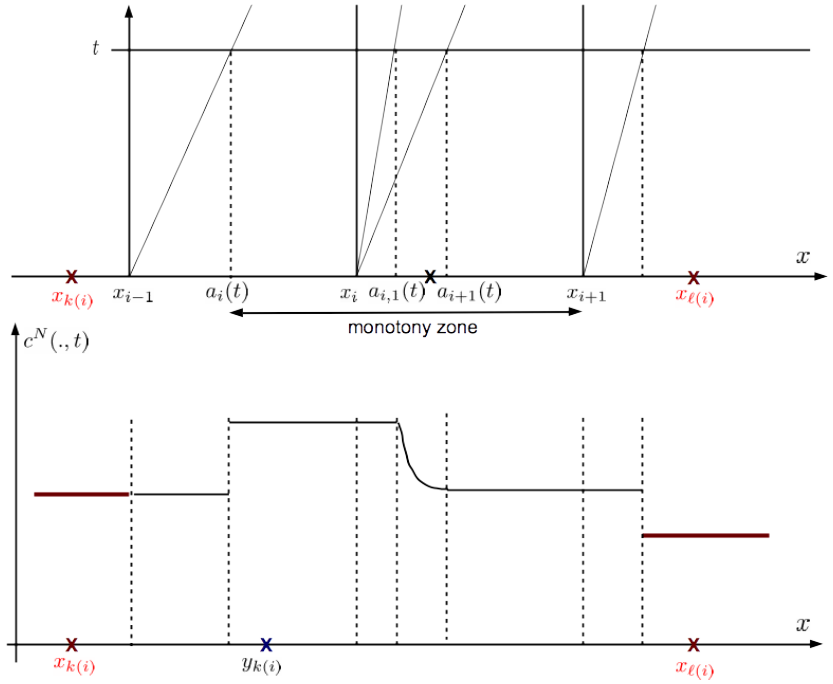

Figure 4: *monotony and subdivisions, case $f" < 0$.*

The last step is the L^2 projection step which produces a piecewise constant function $c^N(t_1,\cdot)$ and we just need to apply Lemma 2.2 below to get

$$TV^s c^N(t_1,\cdot)\{[0,X]\} \le TV^s c_{IB}.$$

Finally we get Proposition 2.4 by induction as in [4, 5]. □

Lemma 2.2 *Let c be a function in $BV^s(\mathbb{R})$ and let $\Delta x > 0$. Then the step function*

$$c^{\Delta x} = \sum_p c_p^{\Delta x}\, \mathbb{1}_{(p\Delta x,(p+1)\Delta x]}, \quad \textit{with} \quad c_p^{\Delta x} = \frac{1}{\Delta x}\int_{p\Delta x}^{(p+1)\Delta x} c(x)\,dx,$$

satisfies

$$TV^s c^{\Delta x} \le TV^s c.$$

The same result holds for any interval.

Proof: for all $p \in \mathbb{N}$ there exists $x_p^{\Delta x}$, $y_p^{\Delta x} \in (p\Delta x,(p+1)\Delta x)$ such that

$$c(x_p^{\Delta x}) \le c_p^{\Delta x} \le c(y_p^{\Delta x}).$$

Let us consider a maximal (for inclusion) finite sequence of indexes p_i, $p_i+1,\cdots,p_{i+1}$ among those corresponding to a monotonic sequence $(c_{p_i}^{\Delta x},\cdots,c_{p_{i+1}}^{\Delta x})$. We set $x_i = x_{p_i}^{\Delta x}$

if the sequence is increasing, $x_i = y_{p_i}^{\Delta x}$ else. The maximality of the sequence of indexes ensures the consistency of this definition. Let σ be a subdivision $\{x_j < x_{j+1} < \cdots < x_{j+k}\}$. By Lemma 2.1 we have clearly $TV^s c[\sigma] \geq TV^s c^{\Delta x}[\sigma]$, but we also have, from the definition of the s-total variation, $TV^s c\{\mathbb{R}\} \geq TV^s c[\sigma]$ and the result follows. □

In the next lemma, the projection step is estimated in $L^{1/s}$ with the BV^s semi-norm. It is enough to get the consistency of the Godunov scheme as in [4, 5]. Moreover, it is used to obtain the Hölder regularity $Lip^s([0,T],\, L^{1/s}([0,X]))$ of the concentration below.

Lemma 2.3 *Let L be a positive constant and $c \in BV^s(0,L)$ with $0 < s \leq 1$. Then,*

$$\int_0^L |c(x) - \overline{c}|^{1/s} dx \leq L \;\; TV^s c\{(0,L)\},$$

where $\overline{c}$ is a mean value of the function c on $(0,L)$, defined by $\dfrac{1}{L}\displaystyle\int_0^L c(x)dx$ or $\dfrac{c(0+)+c(L-)}{2}$.

Proof: there exist $x_-, x_+ \in (0,L)$ such that

$$\inf_{(0,L)} c \leq c(x_-) \leq \overline{c} \leq c(x_+) \leq \sup_{(0,L)} c,$$

so that

$$|c(x) - \overline{c}|^{1/s} \leq \max_{\pm} |c(x) - c(x_\pm)|^{1/s} \leq TV^s c\{(0,L)\}.$$

Integrating over $(0,L)$ gives the expected inequality. □

Proposition 2.5 *For $s \geq 1/3$, we have $\ln u \in L^\infty([0,T]\times[0,X])$. More precisely, there exists a constant C independent of the initial-boundary data such that*

$$|\ln u| \leq |\ln u_b| + 2\|g\|_\infty + C \cdot TV^s c_{IB}.$$

Proof: for a continuous solution, using the Riemann invariant $\ln u + g(c)$ we get

$$|\ln u - \ln u_b| = |g(c) - g(c_b)| \leq 2\|g\|_\infty.$$

Through a shock wave, thanks to Proposition 3.5, we have $\dfrac{u_+}{u_-} = S(c_-, c_+)$ where S is a smooth function. Thanks to the mean value theorem, there exists a true constant γ such that

$$|\ln u_+ - \ln u_-| \leq \gamma |c_+ - c_-|. \tag{31}$$

In the general case, we use the following classical result: shocks curves and rarefaction curves have a second order contact (see Theorem 8.2.2, page 209 in [15]). Then, through a simple $\lambda-$wave

$$\ln u_+ + g(c_+) = \ln u_- + g(c_-) + \mathcal{R}(c_-, c_+)$$

with $\mathcal{R}(c_-, c_+) = \mathcal{O}(|c_+ - c_-|^3)$.

Then, for each wave, we have a new term of order $\mathcal{O}(|c_+ - c_-|^3)$. Hence,

$$|\ln u - \ln u_b| \leq |g(c_b) - g(c)| + C \sum_{waves} |c_+ - c_-|^3,$$

where C is a true constant (depending on the first and second derivatives of the eigenvector associated to the the λ-wave). As $c \in BV^s$ with $s \geq 1/3$, Proposition 2.5 holds thanks to the continuous mapping $BV^s \hookrightarrow BV^{1/3}$. Since $0 \leq c \leq 1$ the constant C is unchanged. □

Now, we conclude the proof of Theorem 2.1. Let $(c^N, u^N)_N$ be the sequence constructed above by the Godunov scheme. The following steps allow to pass to the limit up to a subsequence, still denoted by $(c^N, u^N)_N$. These steps are rather classical except the BV^s aspect.

1. $c^N \in L^\infty([0,T], BV^s([0,X]))$ if the (CFL) condition holds,
2. $|\ln u^N| \leq |\ln u_b| + 2\|g\|_\infty + C \cdot TV^s c_{IB}$ which allows to choose a time step Δt in (30) such that the (CFL) condition is fulfilled,
3. adapting Lemma 4.5 in [4], we have stated in [9] the Hölder estimate in time $Lip^s([0,T],\, L^{1/s}([0,X]))$:

$$\begin{aligned} \forall t_1,\, t_2 \in [0,T], \quad \|c^N(\cdot,t_1) - c^N(\cdot,t_2)\|_{L^{1/s}([0,X])} &= \left(\int_0^X \left| c^N(x,t_1) - c^N(x,t_2) \right|^{1/s} \right)^s \\ &\leq C\left(|t_1 - t_2| + \Delta t \right)^s, \end{aligned} \tag{32}$$

   where the constant C only depends on $TV^s c_{IB}$ and $\|u_b\|_\infty$.

Up to subsequences, $(c^N)_N$ converges strongly towards a function c and $(u^N)_N$ converges weakly towards a function u. This is enough to show that (c,u) is an entropy solution, as in [4, 5]. □

Remark 2.1 Unlike the case of [4, 5, 7] with $s = 1$, we only get a weak trace at the physical boundary $\{x = 0\}$ for the velocity u because we have no longer BV^s estimate.

2.3 Blow-up for $\ln u$ when $s < \dfrac{1}{3}$

For $0 < s < 1$, an explicit example is built to show that we cannot expect a BV_x^s bound for $U = \ln u$ only from inequality (31). Conversely, for $s = 1$ it is true since $TVU \leq \gamma TVc$. A counter-example for $s < 1$ is explicitly stated with two piecewise constant functions (U,c) with values (U_k, c_k) on $(k, k+1)$, $k \in \mathbb{N}$ and satisfying (31), i.e.,

$$|U_{k+1} - U_k| \leq \gamma |c_{k+1} - c_k|.$$

Let σ be such that

$$0 < s < \sigma < 1, \quad c_{k+1} - c_k = \frac{(-1)^k}{k^\sigma} \quad \text{and} \quad U_{k+1} - U_k = |c_{k+1} - c_k|.$$

The function c belongs to $BV^s(0,+\infty)$, then $\displaystyle\sum_k |U_{k+1} - U_k|^{1/s} < +\infty$, but the function U is not bounded, so that $U \notin BV^s(0,+\infty)$.

In the general previous counter-example, the Riemann problem is not solved. The functions U and c are linked through $\lambda-$waves. We generalize a blow-up example built in [8] with ammonia and an inert gas: $f'' > 0$, $h' > 0$ (after exchange of c_1, c_2 with respect to [8]).

In this paper, the piecewise constant initial data $c_0(.)$ does not belong to $BV_x(0, X)$ for a positive fixed X. The following example is built with $c_0(.) \in BV^s(0, X)$ with $0 < s < 1/3$ and $c_0(.) \notin BV^{1/3}(0, X)$. This example shows that $\dfrac{1}{3}$ is the critical exponent as announced in [10]. We impose constant initial data and piecewise constant concentration at the boundary in such a way that Riemann problems at the boundary are alternatively solved by a shock or a rarefaction.

Let us consider a first boundary Riemann problem with data $(c_-,\, c_+,\, u_0)$, $c_- > c_+$ chosen such that the solution is a shock wave and produces a new speed u_1. Next let us consider a second problem with data $(c_+,\, c_-,\, u_1)$ for which the solution is necessarily a rarefaction wave and produces a new speed u_2 with $u_0 \leq u_2 \leq u_1$. We introduce as in [8] the *amplification coefficient* $\mathbf{R}$ defined by

$$u_2 = \mathbf{R}\, u_0.$$

It was shown in [8] that $\mathbf{R}$ only depends on $(c_-,\, c_+)$ and that $\mathbf{R} > 1$ for almost all choices of $(c_-,\, c_+)$ because the system is not in the Temple class ([8]). This is the main ingredient of our example.

Let $N > 1$ be a fixed integer, $0 = x_0 < x_1 < \cdots < x_{2N-1} < X = x_{2N}$, $0 < \underline{c_k} < \overline{c_k} < 1$ such that $\mathbf{R}(\underline{c_k}, \overline{c_k}) > 1$ and $u_0 > 0$. We choose $(\underline{c_k}, \overline{c_k})$ such that $c \notin BV^{1/3}$ but in BV^s for some $s < 1/3$ (see [9] Proposition 2.4) and we can assume that these sequences have a (common) limit. Let c_∞ be a corresponding value of the concentration and also the common limit of the sequences $(\underline{c_k})$ and $(\overline{c_k})$.

Recall that the λ-wave is not linearly degenerate and the system is not in the Temple class (as shown in [8]) thus shock and rarefaction curves have not a contact of order three for all states (c, u) (see for instance [28]). For a well chosen c_∞, there exists $\rho > 0$ such that, near c_∞,

$$\mathbf{R}(\underline{c_k}, \overline{c_k}) \geq 1 + \rho |\underline{c_k} - \overline{c_k}|^3. \tag{33}$$

We solve system (9)-(10) with the following data for $0 < t < T$, $0 < x < X$, $k = 0, 1, \cdots, N-1$:

$$\left\{ \begin{array}{rcl} c(0,t) & = & \overline{c}, \\ u(0,t) & = & u_0, \\ c(x,0) & = & \left\{ \begin{array}{ll} \underline{c_k} & if \quad x_{2k} < x < x_{2k+1}, \\ \overline{c_k} & if \quad x_{2k+1} < x < x_{2k+2}. \end{array} \right. \end{array} \right. \tag{34}$$

Let us denote by u_k the value of $u(x, 0^+)$ when $x_{k-1} < x < x_k$ for a given $k > 0$. With $f'' > 0$ and $h' > 0$ we have N shocks emerging from $((x_{2k}, t = 0))_{k=0}^{N-1}$ and N rarefactions from $((x_{2k+1}, t = 0))_{k=0}^{N-1}$. We have $u_{2k} < u_{2k+2} < u_{2k+1}$. Furthermore,

$$u_{2k+2} = \mathbf{R}_{k+1}\, u_{2k} = \mathbf{R}(\underline{c_k}, \overline{c_k})\, u_{2k}, \;\; u_{2k} = \mathbf{R}_k\, \mathbf{R}_{k-1} \ldots \mathbf{R}_1\, u_0.$$

From inequality (33) and since $c \notin BV^{1/3}$ that sum is infinite: $\sum_k |c_{k+1} - c_k|^3 = +\infty$, which ensures the divergence of the product $\prod_{j=1}^{k} \mathbf{R}_j \to +\infty$ as k goes to infinity, $u_k \to +\infty$, so u is not bounded and does not belong to BV^s.

3 The Lagrangian formulation

In this section we show that system (9)-(10) admits a Lagrangian formulation thanks to a change of variables which is given in subsection 3.1. This formulation is simpler than the Eulerian one because the concentration c satisfies a scalar conservation law. Nevertheless the boundary becomes a free boundary, so we only study the Cauchy problem. We briefly present the hyperbolic features of this system and solve the Riemann Problem. The solution of the Riemann problem is more complicated than the Eulerian one, it is the reason why we obtain the BV^s existence using the Eulerian formulation in section 2.
The Lagrangian formulation will be used in section 4.2 to get a smoothing effect and the uniqueness of the entropy solution.

3.1 Euler-Lagrange change of variables

Following [29, 22, 23, 24] we perform a Euler-Lagrange change of variables under the crucial assumption

$$\inf_{[0,X]\times\mathbb{R}_t} u(x,t) \quad > \quad 0. \tag{35}$$

This assumption is the key assumption to keep the hyperbolicity of system (9)-(10) as it is explained in section 2.1 and in [5].
The following proposition is a particular case of the results in [22] and [24].

Proposition 3.1 (Lagrangian equations for gas chromatography)
Let $X > 0$ and (u, c) be an L^∞ entropy solution of (9)-(10) on $[0, X] \times \mathbb{R}_t$ with initial data c_b, u_b given in (13). Assume the positivity of the incoming velocity (35), then the change of variables : $(x, t) \mapsto (\xi, \tau)$ with $\xi = x$ and $\tau = \mathcal{T}(x, t)$ such that $\mathcal{T}(0, 0) = 0$ and

$$d\tau \quad = \quad u\, dt - h(c)dx, \tag{36}$$

is well-defined and

$$\mathcal{T}(0,t) = \int_0^t u_b(s)\, ds. \tag{37}$$

Let $\mathcal{S} = \mathcal{T}(0,\cdot)^{-1}$: $\mathcal{T}(0, \mathcal{S}(\tau)) = \tau$. The Cauchy problem in Lagrangian variables

writes

$$\begin{aligned}
\partial_\xi c + \partial_\tau(c + f(c)) &= 0, \quad \xi > 0,\ \tau \in \mathbb{R}, && (38)\\
\partial_\xi v - \partial_\tau(v\, h(c)) &= 0, \quad \xi > 0,\ \tau \in \mathbb{R}, && (39)\\
c(0,\tau) &= c_b(\mathcal{S}(\tau)), \qquad \tau \in \mathbb{R}, && (40)\\
v(0,\tau) &= \frac{1}{u_b(\mathcal{S}(\tau))}, \qquad \tau \in \mathbb{R}, && (41)
\end{aligned}$$

where $v = \dfrac{1}{u}$.

We write the derivation of the Lagrangian equations for gas chromatography to be self-contained. The Poincaré's Lemma says that any closed form is an exact form. Then $d\tau$ is well-defined by equation (10). Condition (35) shows that $t \mapsto \mathcal{T}(0,t)$ is an $\mathbb{R}-$homeomorphism. This is also true for any x, the map $\mathcal{T}$ is a Lipschitz transformation.

Relation (36) and assumption (35) yield

$$dt \;=\; v\, d\tau + v\, h(c) d\xi,$$

and then (39) follows. Equation (9) yields the existence of a function z such that

$$dz \;=\; c\,u\,dt - I(c)\,dx = c(d\tau + h(c)\,dx) - I(c)\,dx = c\,d\tau - (I(c) - c\,h(c))d\xi,$$

and then, since the last equality is an exact form, $\partial_\xi c - \partial_\tau(c\,h(c) - I(c)) = 0$. We recall that $f(c) = q_1(c) - c\,h(c)$ so $I(c) - c\,h(c) = c + f(c)$ and (38) follows.

3.2 Hyperbolic features of the Lagrangian system

A natural method is to solve equation (38) which has only one entropy solution and then solve the linear transport equation with "velocity" $-h(c)$. Unfortunately, linear transport equation leads to difficult problems: non existence, non uniqueness, Dirac mass appears with smooth data for too compressive velocity ([1, 2, 3]). We use another strategy and solve the system directly.

The eigenvalues in Lagrangian coordinates are simply

$$\lambda_1(c) = -h(c), \quad \lambda_2(c) = 1 + f'(c).$$

We remark that $1 + f'(c) > -h(c)$. Thus the system is strictly hyperbolic. Indeed, $1 + f'(c) = H(c) - h(c)$ and $H > 1$ imply $1 + f'(c) > -h(c)$. Furthermore, we can check easily that $-h(c)$ is linearly degenerate and the nonlinearity of $1 + f'(c)$ is given by $f''(c)$. Indeed, $1 + f'(c)$ is genuinely nonlinear if and only if $f''(c) \neq 0$ for all $c \in [0,1]$. Then, we assume in this article that $f'' > 0$ everywhere or $f'' < 0$ everywhere.

Since the Euler-Lagrange change of variables conserves the Riemann invariant we obtain the following result.

Proposition 3.2 *For the eigenvalue* $1 + f'(c)$, c *is a Riemann invariant. For the eigenvalue* $-h(c)$, $W = u\,\exp(g(c))$ *is a Riemann invariant.*

The proof of Proposition 3.2 follows from direct computations. In Lagrangian variables [29, 23] the entropies are simply the usual entropies associated to scalar conservation law (38). More precisely,

Proposition 3.3 *The smooth entropy functions for system* (38)-(39) *are* $\psi(c)$ *where* ψ *is any real smooth function. The corresponding entropy flux satisfies* $q'(c) = (1+f'(c))\psi'(c)$.

Notice that entropies are independent of u as in Eulerian variables.

3.3 Riemann Problem for the Lagrangian system

A natural idea to solve 2×2 system (38), (39), would be to solve scalar conservation law (38) and then advection equation (39). But the equation is ill-posed for L^∞ solutions [2]. The solution is not unique and it is generally a measure. We have to control the velocity to perform the Euler-Lagrange change of variables. Instead, a key idea is to resolve the problem as a coupled system.

We solve the Riemann problem in Lagrangian variables.

Proposition 3.4 (Riemann problem)
Assume condition (12) *on the isotherms. Then the Riemann problem with the initial data*

$$c(0,\tau) = c_\pm, \quad v(0,\tau) = v_\pm, \qquad \pm\tau > 0,$$

is solved with two waves associated with eigenvalues $\lambda_1(c) = -h(c) < \lambda_2(c) = 1 + f'(c)$ *and the intermediary constant state* (c_0, u_0) *between the two waves :*

- λ_1-*wave: contact discontinuity,* $c_0 = c_-$,
- λ_2-*wave:* v_0 *is determined by a shock if* $c_- < c_+$ *(in the case* $f'' < 0$*) or a rarefaction wave,*
  - *shock wave:* $\dfrac{v_0}{v_+} = \dfrac{\sigma(c_-,c_+)+h(c_+)}{\sigma(c_-,c_+)+h(c_0)} = S(c_-,c_+)$, *where the shock speed is* $\sigma(c_-,c_+) = 1 + \dfrac{[f(c)]}{[c]}$,
  - *rarefaction wave:* $\dfrac{v_0}{v_+} = \dfrac{G(c_+)}{G(c_-)}$.

Proof: for the linearly degenerate eigenvalue $-h(c)$ we have a contact discontinuity. Since c is the Riemann invariant, it is constant through a λ_1-wave so $c_0 = c_-$.
For the shock waves, we have the same results as in Eulerian coordinates:

$$\begin{aligned} [c + f(c)] &= \sigma[c], \\ -[v\, h(c)] &= \sigma[v]. \end{aligned}$$

with a different slope as in Eulerian coordinates: $\sigma = \dfrac{[f(c)]}{[c]} + 1$. □

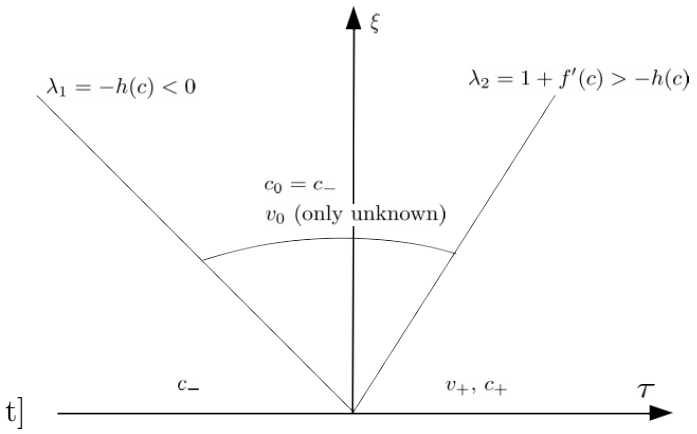

Figure 5: *the Riemann problem, case of a λ_2 shock wave.*

The rarefaction wave is simply given by those of the scalar equation (38). Then, with the Riemann invariant $uG(c)$ we get u.

In [7], some examples are studied to obtain monotonic λ_2- wave curve under convexity assumption on the isotherms. We assume here that $f'' < 0$.

Proposition 3.5 (Monotonic λ_2-waves) *The function $\ln u$ is monotonic through a λ-wave if and only if h is monotonic. Furthermore, $\ln u$ is increasing only if h is increasing.*

Of course, if $h(.)$ is decreasing then $\ln u$ is decreasing through a λ-wave. Many important examples satisfy this monotonicity assumption on h as quoted after Proposition 2.3.

Proof: for a rarefaction wave, with the Riemann invariant $\ln u + g(c)$, we have

$$\ln u_+ - \ln u_- \quad = \quad -\left(g(c_+) - g(c_-)\right).$$

Since $g' = -h'/H$ and $H > 0$, $\ln u$ has the same monotonicity than h.

For a shock wave (see Lemma 5.1 in [7]) we have

$$\frac{u_+}{u_-} \quad = \quad \frac{\sigma + h(c_+)}{\sigma + h(c_-)},$$

with $\sigma = \dfrac{[f]}{[c]} + 1$, $[c] = c_+ - c_-$. Then there exists $\tilde{c} \in (c_-, c_+)$ such that $\sigma = f'(\tilde{c}) + 1$. Moreover, $\sigma = f'(\tilde{c}) + 1 > -h(\tilde{c}) > -h(c_+)$ because we assume for example $h' > 0$. Then $\sigma + h(c_+) > 0$ and we have $u_- > 0$, $u_+ > 0$ then $\sigma + h(c_-) > 0$. Thus, through a shock, $\ln u$ has the same monotony as h. □

4 Consequences of the Lagrangian formulation

In this section, we come back to the Cauchy problem in Lagrangian variables and get both a regularizing effect and a uniqueness result.

4.1 Smoothing effect

The scalar equation for the concentration in Lagrangian variables has a nonlinear flux. The degenerate flux with the genuinely nonlinear assumption on the flux $f'' \neq 0$ gives a smoothing effect for the concentration.

Proposition 4.1 (Regularized concentration)
Let $s \in [1/3, 1]$ and condition (12) on isotherms holds. If $c_b \in BV^s(\mathbb{R}, [0,1])$ and $\ln u_b \in L^\infty(\mathbb{R}, \mathbb{R})$, then the entropy solution (c, u) given by the Godunov scheme on $[0, +\infty) \times \mathbb{R}$ in Theorem 2.1 of the initial value problem (9)-(10) with initial data

$$c(0,t) = c_b(t), \quad u(0,t) = u_b(t), \quad t \in \mathbb{R},$$

becomes more regular in Lagrangian variables:

$$c(\xi,\tau) \in L^\infty_{loc}((0,+\infty)_\xi, BV(\mathbb{R}_\tau)) \cap BV_{loc}((0,+\infty)_\xi \times \mathbb{R}_\tau) \cap Lip(\mathbb{R}_\tau,\, L^1_{loc}((0,+\infty)_\xi)),$$

and also in space-time variables:

$$c(x,t) \in L^\infty_{loc}((0,+\infty)_x, BV(\mathbb{R}_t)) \cap BV_{loc}((0,+\infty)_x \times \mathbb{R}_t) \cap Lip(\mathbb{R}_t,\, L^1_{loc}((0,+\infty)_x)).$$

Proof: in the previous section, the existence of entropy solutions is proved. The Euler-Lagrange change of coordinates is Lipschitz and provides an entropy solution of the Lagrangian formulation (38), (39). The entropy solution of scalar equation (38) with only L^∞ initial data is unique and becomes BV_τ ([18, 20]) for positive ξ. Equation (38) gives the regularity with respect to ξ and the BV regularity with respect to the two variables (ξ, τ). Coming back to the Euler formulation and thanks to the Lipschitz change of variables the concentration is also in BV_t and $BV_{(x,t),loc}$. □

4.2 Uniqueness

System (38)-(39) is composed of a nonlinear equation and a linear equation with a non-smooth coefficient which is $-h(c)$. The non-uniqueness is related to the linear one ([25, 2]) except in the "compressive" case. This last case provides uniqueness for the solution v of equation (39) and then for the Lagrangian formulation.

Proposition 4.2 (Uniqueness for concave isotherm) *Assume $h' > 0$ and $f'' < 0$, $s \in [1/3, 1]$, $c_b \in BV^s(\mathbb{R}, [0,1])$ and $\ln u_b \in L^\infty(\mathbb{R}, \mathbb{R})$. Then, there exists one and only one entropy solution of the initial value problem (9)-(10) with initial data*

$$c(0,t) = c_b(t),\ u(0,t) = u_b(t),\ t \in \mathbb{R}.$$

Proof: Theorem 2.1 provides the existence. The uniqueness is obtained in Lagrangian coordinates. Equation (38) is a scalar conservation law with a unique entropy solution c. Equation (39) is linear $\partial_\xi v + \partial_\tau(a\, v) = 0$ with $a(\xi,\tau) = -h(c)$. The one-sided Lipschitz condition for advection equation (39) is $\partial_x a = -\partial_x h(c) \leq -K$, where K is a constant, ([2]) i.e.

$$\partial_x h(c) \quad \geq \quad K.$$

This inequality imposes the variation of the concentration c through shock waves. The increasing function h has to be nondecreasing through a shock, which is true when $f'' < 0$ (Proposition 3.4). □

The assumptions $h' > 0$ and $f'' < 0$ are related to the isotherms, for instance a concave isotherm (Langmuir) and an inert gas. Other examples are given in [7]. Conversely, for ammonia the assumptions are not valid since $f'' > 0$. Incidentally, ammonia provides an example of blow-up in [8].

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