KINETIC FORMULATION OF A $2 \times 2$ HYPERBOLIC SYSTEM ARISING IN GAS CHROMATOGRAPHY

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Abstract. A particular 2x2 hyperbolic system commonly used in the context of gas-solid chromatography is reformulated as a single kinetic equation using an additional kinetic variable. A kinetic numerical scheme is built from this new formulation and its behavior is tested on solving the Riemann problem in different configurations leading to single or composite waves.

1. Introduction. Since the work of P.-L. Lions, B. Perthame and E. Tadmor [18, 19], it is well known that multidimensional scalar conservation laws and some systems can be formulated as a kinetic equation using an additional kinetic variable. The so-called kinetic formulation of nonlinear hyperbolic systems of conservation laws reduces them to a linear equation on a nonlinear quantity related to the conservative unknowns, moreover it allows to recover all the entropy inequalities. It turns out to be a powerful tool to derive mathematical properties such that regularizing effects or compactness results, invariant domains and also efficient numerical schemes. The method was used by several authors who gave further examples of kinetic formulations: the system of chromatography [15, 22], the Shallow Water system [25], the equations of elastodynamics [24] for instance. The reader may refer to [23] for an overview of the kinetic approach to conservation laws including parabolic scalar conservations laws and some 2x2 hyperbolic systems. The objective of the present work is to apply the machinery of entropy to derive a kinetic formulation for a particular 2x2 hyperbolic system arising in gas chromatography which describes heatless adsorption of a gaseous mixture with two species and already studied by the authors from various points of view [4, 5, 7, 6, 8]. We point out that this formulation in not “purely kinetic” in the sense that the advection velocity contains the macroscopic velocity of the mixture, as in the case of isentropic gas dynamics [19, 23] and in many others physical contexts ([21] for instance), but as we shall see, it is not an obstacle to the derivation of a simple numerical scheme.
due to the particular form of the system. As a first application, we construct such a kinetic numerical scheme, state some of its properties and test it by solving the Riemann problem for some configurations.

The paper is organized as follows. In Section 2, we present the physical context and the model written in its original dimensionless form as a system of material balances equations with a constraint, then we write it in a form more adapted to our study. In Section 3, we recall some basic results of hyperbolicity and entropies for this system. These two sections summarize the results of previous work by the same authors essential to understanding the problem addressed and contain no new result.

In Section 4, we propose and analyze a kinetic formulation of our system. In Section 5 a kinetic scheme is built using the preceding formulation. The last section is devoted to the numerical validation of the scheme, based on the resolution of the Riemann Problem. The exact solution to the Riemann problem for this system (see [5] for instance) is recalled in appendix A.

2. The PSA system. 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 (activated carbon, silica gel, alumina, resin, zeolite...). One of the primary applications of PSA is in the removal of carbon dioxide (CO2) as the final step in the large-scale commercial synthesis of hydrogen (H2) for use in oil refineries and in the production of ammonia (NH3). PSA is used extensively in the production and purification of oxygen for medical uses. Another application of PSA is the separation of carbon dioxide from biogas to increase the methane (CH4) ratio. 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.

As in previous papers by the authors on this subject [4, 5, 6, 8], we focus on a model describing a step of the cyclic process, restricted to isothermal behavior and two species. Working with two species is of course restrictive in view of industrial applications but remains relevant because this corresponds to an important field of applications: for example separation of an He-CO2 mixture [27], of CO2-N2, CO2-CH4 or CO2-H2 mixtures. The kinetic approach that we will propose as well as the numerical scheme that we will deduce from it is specific to this situation and cannot be extended to more than two components.

As examples of more complex situations, the reader will find in [1] a numerical approach to the oxygen enrichment of a mixture of three components (main constituents of air) and in [12] a theoretical and experimental study for the bulk separation of a ternary mixture H2-CH4-CO2.

As in general fixed bed chromatography, each of these two species simultaneously exists under two phases, a gaseous and movable one with concentration \(c_i(t, x)\) or a solid (adsorbed) other with concentration \(q_i(t, x)\), \(1 \leq i \leq 2\). Moreover it is assumed that these concentrations are at equilibrium, i.e. \(q_i(t, x) = q_i^*(c_1, c_2)\) where the so-called isotherms \(q_i^*\) quantify the amount of adsorbate \(i\) on the adsorbent as a function of the partial pressures (or the concentrations, in this isothermal model). The precise form of the isotherms is usually unknown and is experimentally obtained, but there exists empirical models as the linear isotherm due to Henry [28] given by \(q_i^* = K_i c_i\), with \(K_i \geq 0\), semi-empirical models as the Langmuir isotherm [16]
\[ q_i^* = \frac{Q_i K_i c_i}{1 + \sum_{j=1}^{n} K_j c_j}, \text{ with } K_i \geq 0, Q_i > 0 \text{ (see also [17, 18] for instance) and theoretical models as the Brunauer-Emmett-Teller (BET) isotherm [10] which writes, for a single adsorbate with concentration } c, \]
\[ q^*(c) = \frac{Q K c}{(1 + (K - 1) c s)}(1 - \frac{1}{c s}) \text{ with } Q, K > 0 \text{ and } 0 < c_s < 1. \]

Notice that the BET theory is an extension of the Langmuir theory, which is a theory for monolayer molecular adsorption, to multilayer adsorption: gas molecules physically adsorb on a solid in layers infinitely, only interact with adjacent layers and the Langmuir theory can be applied to each layer. This model is mainly suitable for materials with pores larger than a few nanometers.

In each of these models, the isotherms are smooth and increasing with respect to the concentration of the corresponding adsorbate, thus we assume that \( q_i^*(c_1, c_2) \) satisfy
\[ q_i^* \in C^2((0, 1)^2), \quad \frac{\partial q_i^*}{\partial c_i} \geq 0, \quad i \in \{1, 2\}. \] (1)

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, assumed to be constant. The reader can refer for instance to [17].

In [8], the original model, which is nothing more that material balances for two adsorbable components, is written into the dimensionless form:
\[ \partial_t (c_1 + q_1^*(c_1, c_2)) + \partial_x (c_1 u) = 0, \] (2)
\[ \partial_t (c_2 + q_2^*(c_1, c_2)) + \partial_x (c_2 u) = 0, \] (3)
\[ c_1 + c_2 = 1, \] (4)
where \( u \) is the velocity of the gaseous mixture. In this isothermal model, the constraint of constant pressure is achieved through Eq. (4). In the case where an instantaneous equilibrium is not assumed, the corresponding system was studied from both theoretical and numerical points of view by Bourdarias [2, 3].

Setting \( c = c_1 \in [0, 1] \) (then \( c_2 = 1 - c \), \( q_i(c) = q_i^*(c, 1 - c) \), \( i = 1, 2 \), and adding Eqs. (2)-(3), we obtain finally the following system for \( x > 0 \) and \( t > 0 \) which is written in a form (\( x \)-derivative first) justified in the next section:
\[ \begin{cases} \partial_x (u c) + \partial_t I(c) = 0, \\ \partial_x u + \partial_t h(c) = 0, \end{cases} \] (5)
where
\[ h(c) = q_1(c) + q_2(c) \geq 0, \quad I(c) = c + q_1(c). \]
With these notations, the relations (1) read \( q_1^* \geq 0 \geq q_2^* \).

Following [17], we introduce a function which will plays a central role in the nonlinear study of the system, namely,
\[ f(c) = c_2 q_1 - c_1 q_2 = q_1(c) - c h(c). \] (6)

We will also make use of following functions only depending on the isotherms [5]:
\[ H(c) = 1 + q_1^* - c h' = 1 + (1 - c) q_1^* - c q_1^* \geq 1, \] (7)
\[ G(c) = \exp g(c), \] (8)
where $g' = -\frac{h'}{H}$.

3. Hyperbolicity and entropies. To make this paper self-contained, we recall without proofs some results exposed in [5].

As pointed out by Rouchon and al. [26], it is possible to analyze System (5) in terms of hyperbolic system of P.D.E. provided the time and space variables are exchanged: this is why System (5) is presented under this unusual form. In this framework, the vector state is $U = \left( \begin{array}{c} u \\ m \end{array} \right)$ where $m = u c$ is the flow rate of the first species. In this vector, $u$ must be understood as $u(c_1 + c_2)$, that is the total flow rate. The initial-boundary value problem is then System (5) for $x > 0$ and $t > 0$ supplemented by the initial ($x = 0$) and boundary data ($t = 0$):

$$
\begin{align*}
   c(t, 0) &= c_b(t) \in [0, 1], \quad t > 0, \\
   u(t, 0) &= u_b(t) > 0, \quad t > 0, \\
   c(0, x) &= c_0(x) \in [0, 1], \quad x > 0,
\end{align*}
$$

(9)

where

$$0 \leq c_b, c_0 \leq 1,$$

$$0 < \inf \limits_{\mathbb{R}} u_b \leq \sup \limits_{\mathbb{R}} u_b < +\infty.$$

For this system, the first two equations of (9) correspond to the initial data and the last one to the boundary data. That is to say that the variable $x$ is progressive, i.e. 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 $x$. 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.

The eigenvalues of the Jacobian matrix of the flux are 0 and $\lambda = \frac{H(c)}{u}$, thus the system is strictly hyperbolic as long as $u > 0$: we will show in the last section that it is ensured for the solution to the Riemann Problem thanks to the assumption $\inf \limits_{\mathbb{R}} u_b > 0$. Moreover $\lambda$ is genuinely nonlinear in each domain where $f'' \neq 0$. The Riemann invariants are $c$ and $W = u G(c)$ associated to the eigenvalues 0 and $\lambda$ respectively.

We have shown in [5] that there are two families of entropies: $u \psi(c)$ and $\phi(u G(c))$, where $\phi$ and $\psi$ 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 $G'' > 0$ 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 $\partial_x (u G(c)) \geq 0$.

Actually the second family of entropy is included in the first one [5]. It corresponds
to the case when the entropy-flux vanishes (or is constant). More precisely, when \( Q = 0, Q' = 0 \) yields a differential equation for \( \psi \) and then \( \psi = G \).

4. **A kinetic formulation of PSA system.** In this section, we consider weak solutions of System (5) and we give a kinetic formulation. This requires the knowledge of a complete family of supplementary conservation laws or more precisely the weak entropy inequalities. This formulation will be used later to build a kinetic scheme. A second formulation restricted to a convex assumption on isotherms is mentioned in remark.

To have a general kinetic formulation we use the family \( u \psi(c) \), where \( \psi'' \geq 0 \).

Despite the fact that this family is always degenerate convex, this family has the great advantage to be convex without convex assumption on isotherms.

Let us introduce the classic function \( \chi \):

\[
\chi(c, \xi) = \mathbf{1}_{(0,c)}(\xi) = \begin{cases} 
1 & \text{if } 0 < \xi < c, \\
0 & \text{else.} 
\end{cases}
\] (10)

This function enjoys the following simple properties:

\[
\text{supp}(\chi) = [0, c], \quad \int_{\mathbb{R}} \chi(c, \xi) d\xi = c
\]

and

\[
\forall g \in C^1([0,1]), \quad \int_{\mathbb{R}} g'(\xi) \chi(c, \xi) d\xi = g(c) - g(0).
\]

Since \( c \in (0, 1) \) we define \( \chi \) only for \( (c, \xi) \in (0,1) \times (0,1) \) and we have also \( \chi(c, \xi) = \mathbf{1}_{(\xi,1)}(c) \).

Moreover, this function satisfies the fundamental Gibbs property, also called Brenier’s Lemma: let \( S \) be a convex function, \( c \in \mathbb{R} \) and consider the minimization problem

\[
\inf \left\{ \int_0^1 S'(\xi) \phi(c, \xi) d\xi \mid \phi \in L^1(0,1), \ 0 \leq \phi \leq 1 \text{ and } \int_0^1 \phi(c, \xi) d\xi = c \right\}.
\] (11)

Y. Brenier [23, 9] showed that the minimization problem achieves its minimum at \( \phi = \chi \) and that if \( S \) is strictly convex the minimizer is unique.

In order to derive the kinetic formulation of (5), we need to state two technical but easy results.

**Lemma 4.1.** The distribution \( \partial c \chi \) satisfies:

\[
\forall \phi \in C^1_0((0,1)^2), \quad < \phi, \partial c \chi > = \int_0^1 \phi(\xi, c) d\xi.
\]

**Proof.** For all \( \phi \in C^1_0((0,1)^2) \) we have, using \( \chi(c, \xi) = \mathbf{1}_{(\xi,1)}(c) \):

\[
< \phi, \partial c \chi > = - < \partial c \phi, \chi >= - \int_0^1 \int_0^1 \partial_\xi \phi(c, \xi) \chi(c, \xi) d\xi dc
\]

\[
= - \int_0^1 \left( \int_\xi^1 \partial_\xi \phi(c, \xi) dc \right) d\xi
\]

\[
= \int_0^1 \phi(\xi, c) d\xi.
\]
In the following lemma, $H$ is the function defined by Eq. (7). We recall that $H \in C^1(0,1)$.

**Lemma 4.2.** The function $P(c, \xi) = H(\xi) \chi(c, \xi)$ satisfies $\partial_c P = H(c) \partial_c \chi$.

**Proof.** On one hand, using Lemma 4.1

\[
\forall \phi \in C^1((0,1)^2), \quad <\phi(c, \xi), H(c) \partial_c \chi > = < H(c) \phi(c, \xi), \partial_c \chi > = \int_0^1 H(\xi) \phi(\xi, \xi) \, d\xi.
\]

On the other hand,

\[
< \phi(c, \xi), \partial_c P > = < \partial_c \phi(c, \xi), P > = < \partial_c \phi(c, \xi), H(\xi) \chi(c, \xi) >
\]

\[
= - \int_0^1 \int_0^1 H(\xi) \partial_c \phi(c, \xi) \chi(c, \xi) \, dc \, d\xi
\]

\[
= - \int_0^1 H(\xi) \left( \int_0^1 \partial_c \phi(c, \xi) \, dc \right) \, d\xi
\]

\[
= \int_0^1 H(\xi) \phi(\xi, \xi) \, d\xi.
\]

\[\square\]

We are now ready to give our main result:

**Theorem 4.3.** If $(u, c)$ is a weak entropy solution to System (5), then there exists a nonnegative measure $\mu(t, x, \xi)$ such that:

\[
\partial_x (u \psi(c)) + a(\xi) \partial_t \chi(c, \xi) + \partial_t (h(c) \chi(c, \xi)) = \partial_\xi \mu,
\]

where $a$ is given by $a(\xi) = H(\xi) - h(\xi) = 1 + f'(\xi)$.

**Proof.** we begin by obtaining the kinetic formulation (12) by writing entropy inequalities for all $\psi$ such that $\psi'' \geq 0$:

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

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

With Kruzhkov entropies $\psi(c, \xi) = |c - \xi| - |\xi|$ which satisfy

\[
-\frac{1}{2} \partial_\xi \psi(c, \xi) = \chi(c, \xi)
\]

and applying Schwartz’s theorem (stating that non-negative distributions can be represented as Radon measures), we have a nonnegative measure $\mu$ such that:

\[
\partial_x (u \psi(c, \xi)) + \partial_t Q(c, \xi) = -2 \mu(t, x, \xi).
\]

Applying $-\frac{1}{2} \partial_\xi$ on the previous equation we get:

\[
\partial_x (u \chi(c, \xi)) + \partial_t \left( -\frac{1}{2} \partial_\xi Q(c, \xi) \right) = \partial_\xi \mu(t, x, \xi).
\]

So, we have to compute $-\frac{1}{2} \partial_\xi Q(c, \xi)$. Since

\[
\partial_c Q(c, \xi) = H(c) \partial_c \psi(c, \xi) + h'(c) \psi(c, \xi),
\]

we have, applying $-\frac{1}{2} \partial_\xi$ and using Lemma 4.2:

\[
-\frac{1}{2} \partial_\xi \partial_c Q(c, \xi) = H(c) \partial_\xi \chi(c, \xi) + h'(c) \chi(c, \xi)
\]

\[
= \partial_t (H(\xi) \chi(c, \xi)) + h'(c) \chi(c, \xi).
\]
Notice that
\[ \int_0^c h'(y) \chi(y, \xi) \, dy = (h(c) - h(\xi)) \chi(c, \xi), \]
thus we have:
\[ -\frac{1}{2} \partial_\xi Q(c, \xi) = -\frac{1}{2} \partial_\xi Q(0, \xi) + H(\xi) \chi(c, \xi) + (h(c) - h(\xi)) \chi(c, \xi). \]
We get finally
\[ \partial_x (u \chi(c, \xi)) + H(\xi) \partial_x \chi(c, \xi) + \partial_t [ (h(c) - h(\xi)) \chi(c, \xi)] = \partial_\xi \mu. \]

The converse of the previous theorem is the following one:

**Theorem 4.4.** If there exist a positive function \( u \) such that \( \ln u \in L^\infty \), a function \( \phi(t, x, \xi) = \chi(c(t, x), \xi) \) for some function \( c \) and a nonnegative measure \( \mu \) such that
\[ \partial_x (u \phi(t, x, \xi)) + \alpha(\xi) \partial_\phi(t, x, \xi) + \partial_t (h(c) \phi(t, x, \xi)) = \partial_\xi \mu, \]
then \( u, c \) is a weak entropy solution to System (5).

**Proof.** multiplying Equality (14) by \( \partial_\xi \psi \) and integrating over \( (0, \xi) \) we get (13). With (13) we recover easily System (5): first, using \( \psi \equiv \pm 1 \) then \( Q'(c) = \pm h'(c) \) and we recover the second equation of (5), next the choice \( \psi \equiv \pm c \) gives \( Q'(c) = \pm I'(c) \) and we recover the first equation of (5).

**Remark 1.** Writing Eq. (12) under the form
\[ \partial_x (u \chi(c, \xi)) + \partial_t (\alpha(\xi) + h(c)) \chi(c, \xi)) = \partial_\xi \mu \]
we highlight an advection velocity \( \alpha(\xi) + h(c) \) which is is not purely kinetic, as in [19].

For weak solution we can bound the measure \( \mu \) with respect to \( L^\infty \) bound of \( u \).

**Proposition 1 (A priori bound for defect measure).**
If \( u, c \) is a weak entropy solution to System (5) and let \( \mu(t, x, \xi) \) the defect measure satisfying kinetic formulation (12), then there exists a constant \( \alpha > 0 \) depending on \( \| h \|_{L^\infty} \) such that:
\[ \forall T > 0, \forall X > 0, \int_0^T \int_0^X \mu(t, x, \xi) \, dt \, dx \, d\xi \leq \alpha X + T \| u_b \|_{L^\infty(0, T)}. \]

**Proof.** multiplying (12) by \( S'(\xi) \) such that \( S(0) = 0 \), we get
\[ \partial_x (u S'(\xi) \chi(c, \xi)) + \partial_t S'(\xi) (\chi(c, \xi)) + \partial_t (h(c) S'(\xi) \chi(c, \xi)) = S'(\xi) \partial_\xi \mu(t, x, \xi). \]

Integrating by parts the previous equality over \( (0, T) \times (0, X) \times (0, 1) \) we have:
\[ - \int_0^T \int_0^X S''(c) \, \mu \, dt \, dx \, d\xi = \int_0^T [u(t, X) S(c(t, X)) \]
\[ - u_b(t) S(c_b(t))] \, dt + \int_0^X (A(c)(T, x) - A(c_0)(x)) \, dx \]
where \( A(c) = \int_0^c a(\xi) S'(\xi) \, d\xi + h(c) S(c) \). Since \( 0 \leq c \leq 1 \), we have only to estimate \( u(t, X) \). To control \( \int_0^T u(t, X) \, dt \) we use second equation of System (5): \( \partial_x u = -\partial_t h(c) \) and nonnegativity of \( h \), then:
\[ \int_0^T u(t,X) \, dt = \int_0^T u_b(t) \, dt + \int_0^X (h(c_0(x)) - h(c(T,x))) \, dx \leq \int_0^T u_b(t) \, dt + \int_0^X h(c_0(x)) \, dx. \]

With \( S(c) = c^2/2 \), a constant \( \alpha \) depending only on the supremum of \( A \) and \( h \) on \((0,1)\) and the last inequality we can conclude the proof.

\textbf{Remark 2.} There exists a second kinetic formulation, not used in this paper, based on the following property: if \( G'' > 0 \), for all weak entropy solutions and all \( \phi \) such that the mapping \( (u,m) \mapsto \phi(\ln(u) + g(m/u)) \) is convex, see Section 3, we have \( \partial_x (\phi(uG(c))) \leq 0 \).

Unfortunately these kind of entropy is related with convexity or not of isotherms. Furthermore we cannot expect to recover all System (5) (but if \( G'' > 0 \) we must have the Lax entropy condition).

5. A kinetic scheme for the PSA system. In this section a kinetic scheme related to the kinetic formulation (14) is proposed. If the velocity \( u \) is frozen then the kinetic formulation seems only related to the concentration \( c \). Thus a kinetic scheme for scalar conservation laws can be used except that the macroscopic variable \( c \) appears in the kinetic velocity. Then, an important step is to update the velocity. To be consistent with the PDE, the second equation of PSA System 5 is used. This scheme, presented in Section 5.1, enjoys some mathematical properties: maximum principle in Section 5.2, \( BV \) estimates in Section 5.3 and the scheme satisfies entropy inequality in Section 5.4. Finally the scheme is tested with exact solutions of some Riemann problems and many isotherms in Section 6.

5.1. The kinetic scheme. Let \( T > 0 \) be the duration of the simulated process. The interval \([0,T]\) is divided in \( N \) intervals \((t_{i-1/2},t_{i+1/2})\) \((t_{1/2} = 0)\) with same length \( \Delta t = T/N \), centered in \( t_i \). At each time step a new spatial mesh \([x_n,x_{n+1}]\) \((x_0 = 0)\) with length \( \Delta x^n \) is defined, according to some CFL type condition. The discrete unknowns \((u_i^n,c_i^n)\) with \( n \in \mathbb{N}^* \) and \( 1 \leq i \leq N \) are the approximations of the velocity and the concentration, respectively, at \( x = x_n \) in the temporal mesh \( T_{e_i} = (t_{i-1/2},t_{i+1/2}) \).

The initial and boundary data are taken into account setting:

\[ c_0^n = \int_{x_n}^{x_{n+1}} c_0(x) \, dx, \quad 0 \leq n \leq N - 1, \quad (15) \]

\[ u_0^i = \int_{T_{e_i}} u_b(t) \, dt, \quad c_0^i = \int_{T_{e_i}} c_b(t) \, dt, \quad i \in \mathbb{N}. \quad (16) \]

Let \( I \geq 2 \) be an integer. Given \((u_i^n,c_i^n)\) for \( i = 1, \ldots, I \), we denote \( u^n \) (resp. \( c^n \)) the piecewise function with value \( u_i^n \) (resp. \( c_i^n \)) on \((t_{i-1/2},t_{i+1/2})\) and we introduce the following transport equation related to (14) on \([x_n,x_{n+1}]\) (with \( x \) as the evolution variable):
\[ \partial_t (u^n(t) \phi(t, x, \xi)) + \partial_x ((a(\xi) + h(c^n(t))) \phi(t, x, \xi)) = 0 \tag{17} \]

with \( t > 0, \ x_n \leq x < x_{n+1}, \ \xi \in \mathbb{R} \)

and \( \phi(t, x_n, \xi) = \chi(c^n(t), \xi) \quad t > 0, \ \xi \in \mathbb{R} \). \tag{18}

This equation is solved numerically, using a standard explicit upwind finite volume scheme. More precisely, we set, for each \( \xi \leq b \) effective in all the columns for \( 0 \leq t \leq T \) of System (5): Equation (20) with respect to the first equation of System (5) is of order 1 in time and space.

Thus \( \phi_{i}^{n+1}(\xi) \) is given by the following scheme:

\[
\Delta t u_i^n \left( \phi_{i}^{n+1}(\xi) - \chi_i^n(\xi) \right) + a(\xi) \Delta x^n \left( \phi_{i+1/2}^n(\xi) - \phi_{i-1/2}^n(\xi) \right) + \Delta x^n h(c_i^n) (\chi_i^n(\xi) - \chi_{i-1}^n(\xi)) = 0, \tag{19} \]

with

\[ \phi_{i+1/2}^n(\xi) = \begin{cases} 
\chi_i^n(\xi) & \text{if } a(\xi) \geq 0, \\
\chi_{i+1}^n(\xi) & \text{if } a(\xi) < 0,
\end{cases} \]

i.e.

\[ a(\xi) \phi_{i+1/2}^n(\xi) = a^+(\xi) \chi_i^n(\xi) - a^-(\xi) \chi_{i+1}^n(\xi) \]

where \( a^+ = \max(a, 0) \) and \( a^- = -\min(a, 0) \).

Notice that \( \phi_{i}^{n+1}(\xi) \) is no longer a Gibbs equilibrium, i.e. a \( \chi \) function. We recover such an equilibrium setting \( c_{i}^{n+1} = \int_{\mathbb{R}} \phi_{i}^{n+1}(\xi) \, d\xi \) and thus getting \( \chi_{i}^{n+1} \).

At the macroscopic level, integrating (17) with respect to the kinetic variable \( \xi \) we get:

\[
c_{i}^{n+1} = c_{i}^{n} - \chi_{i}^{n} \left\{ (A^+(c_{i}^{n}) - A^+(c_{i-1}^{n})) \\
- (A^-(c_{i+1}^{n}) - A^-(c_{i}^{n})) + h(c_{i}^{n}) (c_{i}^{n} - c_{i-1}^{n}) \right\} \tag{20}
\]

where we have set, as long as \( u_i^n > 0 \):

\[ \chi_{i}^{n} = \frac{\Delta x^n}{u_i^n \Delta t}, \quad A^+(c) = \int_{c}^{\infty} a^+(\xi) \, d\xi. \tag{21} \]

Finally, we update the velocity \( u \) applying a classical finite difference scheme to the second equation of System (5):

\[
u_i^{n+1} = u_i^n - \frac{\Delta x^n}{2\Delta t} (h(c_{i+1}^{n}) - h(c_{i-1}^{n})). \tag{22} \]

**Remark 3.** A simple calculation (Taylor expansions for a smooth solution \((c, u)\)) shows that the theoretical consistency error for the numerical scheme given by Equation (20) with respect to the first equation of System (5) is of order 1 in time and space.

Notice that \((15)-(16)-(21)-(20)-(22)\) allow to compute \((u_i^{n+1}, c_i^{n+1})\) for \( i = 1 \) to \( I - 1 \) only, because the sign of \( a \) is not a priori known, thus the computation will be effective in all the columns for \( 0 \leq t \leq T = (I - M + 1) \Delta t \) if \( M \) is the number of spatial meshes. We have thus to extend the temporal domain and the functions \( u_b, c_b \) in a suitable way, \( M \) being estimated following Remark 4.

In the sequel we note (KS) the kinetic scheme defined by \((15)-(16)-(21)-(20)-(22)\).
5.2. $L^\infty$ estimates.

**Proposition 2.** Assume that $u_b \geq \alpha$ for some constant $\alpha > 0$. As long as $u^n_i > 0$, if $\Delta x^+$ satisfies at each time step the CFL type condition

$$
(\| h \|_\infty + 2 \| a \|_\infty) \Delta x^n \leq \min_i (u^n_i) \Delta t,
$$

(23)

then we have the following $L^\infty$ estimates:

$$
0 \leq \phi^n_i \leq 1, \quad 0 \leq c^n_i \leq \max\{\| c_b \|_\infty, \| c_0 \|_\infty \} \leq 1.
$$

(24)

In (23), the $L^\infty$ norms are relative to $[0,1]$.

**Proof.** writing (19) under the form

$$
\phi^n_i+1(\xi) = (1 - \lambda^n_i (|a(\xi)| + h(c^n_i))) \chi^n_i(\xi) + \lambda^n_i (a^+(\xi) + h(c^n_i)) \chi^n_{i-1}(\xi) + \lambda^n_i a^-(\xi) \chi^n_{i+1}(\xi)
$$

we obtain $\phi^n_i+1(\xi)$ as a convex combination of $\chi^n_{i-1}(\xi)$, $\chi^n_i(\xi)$ and $\chi^n_{i+1}(\xi)$ as soon as (23) is satisfied. Thus the first inequality of (24) holds by induction. In the same manner we can write (20) as

$$
c^n_{i+1} = \left(1 - \lambda^n_i \left( p^n_{i-1/2} + p^n_{i+1/2} + h(c^n_i) \right) \right) c^n_i + \lambda^n_i (p^n_{i-1/2} + h(c^n_i)) c^n_{i-1}
$$

$$
+ \lambda^n_i p^n_{i+1/2} c^n_{i+1},
$$

where $p^n_{i-1/2} = \frac{A^+(c^n_{i-1}) - A^+(c^n_{i+1})}{c^n_i - c^n_{i-1}}$ and $p^n_{i+1/2} = \frac{A^-(c^n_{i+1}) - A^-(c^n_i)}{c^n_{i+1} - c^n_i}$ satisfy:

$$
0 \leq p^n_{i-1/2} \leq \| a^+ \|_\infty \quad \text{and} \quad 0 \leq p^n_{i+1/2} \leq \| a^- \|_\infty
$$

and the second inequality of (24) holds by induction since $\| a^+ \|_\infty + \| a^- \|_\infty \leq 2 \| a \|_\infty$. \hfill \square

**Remark 4.** The previous result is not fully satisfactory because we are not currently able to give a positive lower bound for $u$ as with the Godunov scheme [5]. Notice however that in the case of smooth solutions, we could choose to update the velocity using the Riemann invariant $W$, that is setting

$$
u^{n+1}_i G(c^{n+1}_i) = u^n_i G(c^n_i).
$$

(25)

In this case we get immediately by induction: $u^n_i \geq \alpha \frac{\inf_{[0,1]} G}{\| G \|_\infty}$. Then we can use the uniform CFL condition:

$$
\| G \|_\infty (\| h \|_\infty + 2 \| a \|_\infty) \Delta x \leq \alpha \Delta t \inf_{[0,1]} G,
$$

and of course (24) holds, but this is no longer relevant in the general case: due to the presence of shock wave, the equality $\partial_x W = 0$ becomes a strict inequality. Thus, such a computation on $u$ through a shock wave is not consistent.
5.3. **BV estimates.** This scheme is a TVD scheme. Let us define the total variation (with respect to the time variable) of \((c^n_i)_{i \in \mathbb{N}}\) by

\[
TV^n(c) = \sum_{i=0}^{\infty} |\Delta c^n_{i+1/2}|, \quad \text{with} \quad \Delta c^n_{i+1/2} = c^n_{i+1} - c^n_{i}.
\]

**Proposition 3.** The kinetic scheme (KS) is total variation diminishing, that is

\[
\forall n \in \mathbb{N} \quad TV^{n+1}(c) \leq TV^n(c) + TVc_0,
\]

under the (CFL) condition (23).

**Proof.** We have just to show that \(c^n_i\) may be written under an incremental form (see for instance [13, 14]). Now we have:

\[
c^n_{i+1} = c^n_{i} + A^n_{i+1/2} \Delta c^n_{i+1/2} - B^n_{i+1/2} \Delta c^n_{i-1/2}
\]

with

\[
A^n_{i+1/2} = \lambda^n_i p^n_{i+1/2} \quad \text{and} \quad B^n_{i+1/2} = \lambda^n_i \left( h(c^n_i) + p^n_{i-1/2} \right).
\]

So it is easy to verify that under the condition (23) we have

\[
A^n_{i+1/2} \geq 0, \quad B^n_{i+1/2} \geq 0, \quad \text{and} \quad A^n_{i+1/2} + B^n_{i+1/2} \leq 1
\]

which ensures the incremental form for \(c^n_i\) and thus concludes the proof. \(\square\)

5.4. **Discrete entropy inequalities.** An important requirement for the scheme is to satisfy some entropy inequalities.

**Proposition 4.** The discrete unknowns \((u^n_i, c^n_i)\) satisfy the following discrete entropy inequality, where \(\psi\) is any real smooth function such that \(\psi'^{\pm} \geq 0\):

\[
u^n_i \psi(c^{n+1}_i) \leq u^n_i \psi(c^n_i) - \frac{\Delta x^n}{\Delta t} \left( \Phi^n_{i+1/2} - \Phi^n_{i-1/2} \right) - \frac{\Delta x^n}{\Delta t} h(c^n_i) \left( \psi(c^n_i) - \psi(c^n_{i-1}) \right)
\]

where \(\Phi^n_{i+1/2} = \Phi^+(c^n_i) - \Phi^-(c^n_{i+1})\) with \(\Phi^\pm = \int \psi' a^\pm\).

**Proof.** Inequality (26) arises mutiplying (19) by \(\psi'(\xi)\), integrating over \(\mathbb{R}\) with respect to \(\xi\) and applying Brenier’s lemma (see Section 4) thanks to the \(L^\infty\) estimate (24) on \(c^{n+1}_i(\xi)\). \(\square\)

6. **The kinetic scheme and the Riemann problem.** In this section our aim is to test the ability of the kinetic scheme to select the entropy solution of the Riemann problem for various choices of isotherms following [17]. The notations \((c^-, c^+, \ldots)\) are those of appendix A. In particular, the BET isotherm with one inflexion point leads to composite waves which we will see that they are properly computed by the scheme. For these numerical experiments, the number of temporal meshes was chosen (after various tests) in order to make a compromise between the computation time (a few minutes), the precision in the position of the fronts and the minimization of the diffusive effects. Notice that we do not pretend, in this work, to apply our scheme to experimental configurations and our approach is qualitative but the different cases correspond nevertheless to common and fundamental situations such as adsorption or desorption steps.

We will present a study of the error on the concentration \(c\) in the case of a contact discontinuity and a regular solution (rarefaction wave with the Langmuir isotherm). For this purpose we will compute the relative error \(Erel = \frac{\|c_{num} - c_{ex}\|_1}{\|c_{ex}\|_1}\) in the discrete \(L^1\) norm, where \(c_{num}\) is the numerical solution and \(c_{ex}\) is the exact solution of the Riemann problem. To make a self-contained paper, we recall in
appendix A the solution to the Riemann Problem [5], moreover the hyperbolicity condition \( u > 0 \) is ensured for this solution by Proposition 8.

6.1. **One adsorbable component and inert gas.** In this subsection we compare the exact solution to a Riemann problem with the approximation given by the kinetic scheme in the case of one active gas and one inert gas, with various isotherms. In the following numerical examples we successively consider the case of a contact discontinuity and a composite wave.

Assume that \( q_2^* = 0 \): the first component is the only active gas. The length of the column is \( L = 0.1 \).

6.1.1. **Contact discontinuity.** In this first test case, as in [17], we use the following isotherm

\[
q_1(c) = K_1 \frac{c}{1 - c}
\]

for which the function \( f \) is linear: \( f(c) = q_1(c) (1-c) = K_1 c \). This isotherm presents a singularity for \( c = 1 \) but we use initial and boundary data (defined in Eq. (9)) in \((0, 1)\) for the concentration and the maximum principle on \( c \) stated in [5], namely

\[
0 \leq \min(\inf c_b, \inf c_0) \leq c \leq \max(\sup c_b, \sup c_0) \leq 1,
\]

guarantees that the solution remains in \((0, 1)\) for all time.

According to Prop. (7), the Riemann Problem in the \((t, x)\) plane is solved by a contact discontinuity connecting \((c-, u^-) = (0, 0.2)\) to \((c^-, u^0)\), with \( u^0 \approx 0.10385 \), followed by a contact discontinuity (due to the linearity of \( f \)) connecting \((c^-, u^0)\) to \((c^+, u^+) = (0.7, 0.2)\).

In this simulation we have set \( K_1 = 1 \) and we used 200 temporal meshes. The comparison with the exact solution is presented Fig. 1. One can see Fig. 2 that the scheme is approximately of order 0.64 in this case. In Fig. 3 we give the CPU time for an increasing number \( N \) of temporal meshes, the computations being performed on a desktop computer equipped with a 3.4 GHz Intel Core i7 processor, with the MATLAB software.

6.1.2. **Adsorption step with the BET isotherm: Combined waves.** The so-called BET isotherm, in our adimensional variables, is given by:

\[
q_1(c) = \frac{Q K c}{1 + (K - \frac{1}{c_s}) c (1 - \frac{1}{c_s})}
\]

with \( 0 < c_s < 1 \).

In this simulation we have set \( Q = 1 \), \( K = 10 \), \( \frac{1}{c_s} = 1.3 \) and we used 30 temporal meshes. The choice of parameters in \( q_1 \) is done in order to obtain a corresponding function \( f \) with an inflection point more easily visible in Fig. 4 below. The Riemann Problem in the \((t, x)\) plane is solved by a contact discontinuity connecting \((c^-, u^-) = (0.1, 1)\) to \((c^-, u^0)\), with \( u^0 \approx 0.39701 \), followed by a shock connecting \((c^-, u^0)\) to \((c^*, u^*) \approx (0.41546, 0.54985)\) and a rarefaction connecting \((c^*, u^*)\) to \((c^+, u^+) = (0.7, 1)\). The results are given Fig. 5 and we observe that the Riemann Problem in this more complex situation is correctly solved.

6.2. **Two adsorbable components with the binary Langmuir isotherm.** In this subsection, we assume that the two gases are active and that the process is driven by the binary Langmuir isotherm:

\[
q_i^*(c_1, c_2) = \frac{Q_i K_i c_i}{1 + K_1 c_1 + K_2 c_2}, \text{ with } K_i > 0, Q_i > 0, \quad i = 1, 2.
\]
The following numerical examples show the accuracy of the scheme for contact shock and rarefaction waves.
The length of the column is $L = 0.1$. In this simulation, we have set $Q_1 = Q_2 = 1$, $K_1 = 30$ and $K_2 = 10$: with these values we get a concave function $f$ (see Fig. 6 below).

The first case, with $c^- < c^+$ (adsorption step) is solved by a contact discontinuity connecting $(c^-, u^-) = (0.2, 0.2)$ to $(c^-, u^0)$, with $u^0 \approx 0.19715$, followed by a shock connecting $(c^-, u^0)$ to $(c^+, u^+) = (0.7, 0.2)$. We used 50 temporal meshes and the results are given Fig. 7.

The second case, with $c^- > c^+$ (desorption step) is solved by a contact discontinuity connecting $(c^-, u^-) = (0.7, 0.2)$ to $(c^-, u^0)$, with $u^0 \approx 0.20289$, followed by a rarefaction connecting $(c^-, u^0)$ to $(c^+, u^+) = (0.2, 0.2)$. We used 200 time meshes and the results are given Fig. 8: the concentration $c$ is smooth and the scheme is
7. Conclusion. We have presented a kinetic formulation of the PSA system, written in an adimensional form, which is used in the context of chemical engineering. This formulation, using an additional real variable, consists in a single equation which contains, in some sense, the whole system of two equations and all the entropy inequalities. As a first application, we have built a kinetic scheme, easy to implement and enjoying good properties (positivity and entropy inequality). It has been tested on the resolution of the Riemann problem in various configurations, including the case of an isotherm with at least one inflection point, as the BET isotherm, leading to composite waves. Contact discontinuities are difficult to estimate with accuracy, [23] p. 177. It goes without saying that composite waves
Figure 8. Desorption step (bottom) with the binary Langmuir isotherm. Exact and computed solutions at $t = 1$ along the column $0 \leq x \leq 0.1$

Figure 9. Rarefaction: $-\log(E_{rel})$ vs $-\log(\Delta t)$

Figure 10. Rarefaction: CPU time vs $N$

are more difficult to compute. Here, the proposed kinetic scheme is capable of recovering the good contact wave and the good composite wave with a sufficiently
small mesh. The good agreement with the analytical solution is an argument for convergence and entropic character of the scheme.

Appendix A. Exact solution to the Riemann problem. We consider the following Riemann problem:

\[
\begin{align*}
\partial_x u + \partial_t h(c) &= 0, \\
\partial_x (uc) + \partial_t I(c) &= 0,
\end{align*}
\]

\[c(0, x) = c^- \in [0, 1], \quad x > 0, \quad \left\{ \begin{array}{c} c(t, 0) = c^+ \in [0, 1], \quad t > 0 \\
u(t, 0) = u^+ > 0, \end{array} \right. \]

and we search a selfsimilar solution, i.e. \(c(t, x) = C(z), \ u(t, x) = U(z)\) with \(z = \frac{t}{x} > 0\).

**Figure 11.** Data for the Riemann problem

The exact solution is computed using the following results stated for instance in [5].

**Proposition 5 (Rarefaction waves).** Any smooth non-constant self-similar solution \((C(z), U(z))\) of (27) in an open domain \(\Omega = \{0 \leq \alpha < z < \beta\}\) where \(f''(C(z))\) does not vanish, satisfies:

\[
\begin{align*}
\frac{dC}{dz} &= \frac{H(C)}{zf''(C)}, \\
U(z) &= \frac{H(C)}{z}.
\end{align*}
\]

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

**Corollary 1.** Assume for instance that \(0 \leq \alpha < c^- < c^+ < b \leq 1\) and \(f'' > 0\) in \([a, b]\). Then the only smooth self-similar solution to (27)-(28) is such that:

\[
\begin{align*}
C(z) &= c^-, & 0 < z < z^-, \\
\frac{dC}{dz} &= \frac{H(C)}{zf''(C)}, & z^- < z < z^+ \\
U(z) &= \frac{H(C)}{z}, & z^+ < z,
\end{align*}
\]
where
\[ z^+ = \frac{H(c^+)}{u^+}, \quad z^- = z^+ e^{-\Phi(c^+)} \]
with \( \Phi(c) = \int_{c^-}^{c^+} \frac{f''(\xi)}{H(\xi)} \, d\xi \). Moreover \( U \) is given by:
\[
\begin{cases}
U(z) = u^0, & 0 < z < z^-, \\
U(z) = \frac{H(C(z))}{z^+}, & z^- < z < z^+, \\
U(z) = z^+, & z^+ < z.
\end{cases}
\]

where \( u^0 = \frac{H(c^-)}{z^-} \).

Remark 5. It appears that \( c \) is always monotone along a rarefaction wave but no longer \( u \) because the sign of \( h' \) may change. Indeed the Riemann invariant \( w = \ln u + g(c) \) is constant along such a wave and \( g', h' \) have opposite signs. However notice that in the case where one gas is inert, \( u \) is monotone (see also [4]).

We are looking now for admissible shocks in the sense of Liu [20].

Proposition 6 (\( \lambda \)-shock waves). If \((c^-, c^+)\) satisfies the following admissibility condition equivalent to the Liu entropy-condition:

\[ \frac{f(c^+) - f(c^-)}{c^+ - c^-} \leq \frac{f(c) - f(c^-)}{c - c^-}, \]

then the Riemann problem (27)-(28) is solved by a shock wave defined as
\[
C(z) = \begin{cases}
c^- & \text{if } 0 < z < s, \\
c^+ & \text{if } s < z,
\end{cases} \quad U(z) = \begin{cases}
u^0 & \text{if } 0 < z < s, \\
u^+ & \text{if } s < z,
\end{cases}
\]

where \( u^0 \) and the speed \( s \) of the shock are obtained through
\[ u^0([I] - c^- [h]) = u^+([I] - c^+ [h]), \quad \text{and } s = \frac{[h]}{[u]}, \]

(29)

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

Proposition 7. Two states \( U^- \) and \( U^+ \) are connected by a contact discontinuity if and only if \( c^- = c^+ \) (with of course \( u^- \neq u^+ \)), or \( c^- \neq c^+ \) and \( f \) affine between \( c^- \) and \( c^+ \).

Finally, concerning the Riemann problem, we make use of the following wave fan admissibility criterion (see [11] for instance): the fan is admissible if each one of its shocks, individually, satisfies the Liu shock admissibility criterion.

Then, in view of the previous results, we get the solution to the Riemann problem (27)-(28) for \( c \) in a very simple way, similar to the scalar case with flux \( f \).

Case \( c^- < c^+ \): we consider the lower convex envelope \( f_c \) of the function \( f \) (see Fig. 12, left). On the subintervals where \( f \) is strictly convex (then \( f = f_c \) ) we get a rarefaction wave according to Corollary 1. Elsewhere we get admissible shock waves (or contact discontinuities if \( f \) is affine).

Case \( c^- > c^+ \): we use the upper convex envelope \( f^c \) (see Fig. 12, right) and get rarefaction waves where \( f \) is strictly concave.

The subsection is concluded by a new general result about the positivity of the velocity which improves a similar result in [8]. In other words the region \( \{0 < u, 0 \leq c \leq 1\} \) is an invariant domain for Riemann Problems. Notice that the positivity of \( u \) is mandatory to keep the system hyperbolic, and the velocity can blow up [6].
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Figure 12. Shocks chords are shown as dashed lines. On the left \( c^- \) is connected to \( c^+ \) via a shock (S), a rarefaction wave (R) and a shock. On the right, \( c^- \) is connected to \( c^+ \) via a shock and a rarefaction wave.

**Proposition 8.** Assume that \( f \) has a finite number of inflexion points, then the solution to the Riemann Problem with \( u^+ > 0 \) involves a positive velocity.

**Proof.** with the previous results, the solution to the Riemann Problem consists in a finite sequence of simple waves and it remains to show that the result holds for a simple wave. In the case of a rarefaction wave we have, using (25), 
\[
0 < u^+ = u^+ \frac{G(c^+)}{G(c^-)} < 0.
\]
In the case of a shock wave, we rewrite (29) as follows:
\[
u^0 = \begin{cases} 
A & 
\begin{pmatrix}
1 + \frac{q_1}{c} (1 - c^-) - c^- \frac{q_2}{c} \\
1 + \frac{q_1}{c} (1 - c^+) - c^+ \frac{q_2}{c}
\end{pmatrix} 
\end{cases}
\]
We have \( \frac{q_2}{c} < 0 < \frac{q_1}{c} \), thanks to (1), and \( 0 \leq c \leq 1 \) thus \( A, B \geq 1 \) and \( u^0 > 0 \).

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