Blow up at the hyperbolic boundary for a 2x2 system arising from chemical engineering

Christian Bourdarias, Marguerite GISCLON, Stéphane Junca

University of Savoie, LAMA, UMR-CNRS-5127

Université de Nice Sophia-Antipolis, Labo JAD & Epi COFFEE INRIA

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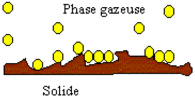
What is it ?

Chromatography gas-solid :

a technic for analyzing a gaseous mixture

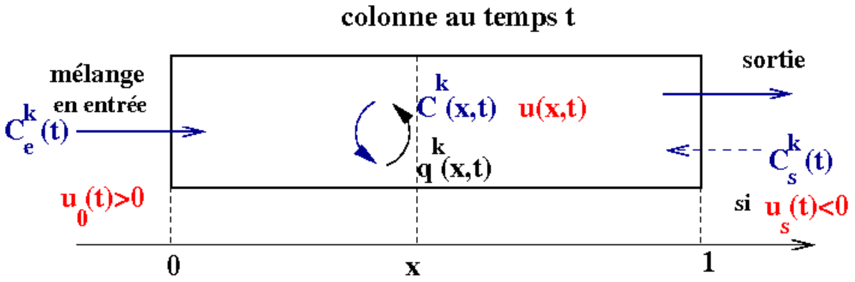


The mixture analysed is vaporised at the entrance of a column that contains a solid substance (the absorber) called the stationary phase and then it is transported across it by a gas carrier. The gas carrier (or gas vector) is the mobile phase. In most cases it has to be inerted vis a vis the solutes and the stationary phase.

Unknowns

During the processus, d species exist together under 2 phases

- one gas phase of concentration c_i and moving with speed u
- one solid (adsorbed) with concentration q_i^*



We define by u the speed of a tracer that is inert in the column. This is a measure of the speed of the flow across the column. **In general this speed can not be considered constant.**

Non linear chromatography

Chemical assumptions

- constant temperature
- 1D model, $x \in \mathbb{R}_+$
- negligeable axial diffusion
- perfect gas
- instantaneous exchange

Prospects

- nonisothermal model
- validity of the model
- relaxation

Equations

Mass conservation :

$$\partial_t(c_i + \mathbf{q_i^*}) + \partial_x(u\, c_i) = 0, \quad 1 \leq i \leq d$$

$\mathbf{q_i^*}$ depends on all c_i :

$$\mathbf{q_i^*} = \mathbf{q_i^*}(c_1, \cdots, c_d)$$

$\mathbf{q_i^*}$ is the i^{th} isothermal law given by the experiments (chemistery)

Classic isotherms

Linear isotherm : $\mathbf{q_i^*} = K_i\, c_i,$ avec $K_i \geq 0$

Langmuir isotherm :

$$\mathbf{q_i^*} = \frac{Q_i\, K_i\, c_i}{1 + \sum_{j=1}^{d} K_j\, c_j}, \text{ with } K_i \geq 0, Q_i > 0$$

BET isotherm : one active gas and one inert gas ($q_2^* = 0$)

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

Sorption effect

Unknowns : velocity u, gazeous concentrations c_i

In gas-solid chromatography, the velocity u is not constant :
it depends on the mixture composition, which depends on mass transfer between phases.
The velocity of the mixture has to be found in order to achieve a given pressure (or density in the isothermal model). The sorption effect is taken into account through a constraint

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

ρ : the given total density of the mixture (the same in the column)

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$\rho \equiv 1$ and $x \in \mathbb{R}_+$:

$$\begin{aligned} \partial_t(c_1 + \mathbf{q_1^*}(c_1, c_2)) + \partial_x(u\, c_1) &= 0 \qquad (1) \\ \partial_t(c_2 + \mathbf{q_2^*}(c_1, c_2)) + \partial_x(u\, c_2) &= 0 \qquad (2) \\ c_1 + c_2 &= 1 \qquad (3) \end{aligned}$$

Let $c = c_1$ and $\mathbf{q_i}(c) = \mathbf{q_i^*}(c, 1 - c) \quad i = 1, 2$

(1) + (2) yields with (3) :

$$\partial_t(\mathbf{q_1}(c) + \mathbf{q_2}(c)) + \partial_x u = 0$$

N.B. : isotherm properties : $q_1' = \dfrac{dq_1}{dc} \geq 0$ and $q_2' = \dfrac{dq_2}{dc} \leq 0$

The 2×2 system

$$
\left\{
\begin{array}{l}
\partial_t(c + q_1(c)) + \partial_x(u\,c) = 0 \\
\partial_t(\underbrace{q_1(c) + q_2(c)}_{= h(c)}) \quad + \partial_x u = 0
\end{array}
\right.
$$

Initial boundary values :

$$
\left\{
\begin{array}{rcl}
c(0,x) & = & c_0(x) \in [0,1], \quad x > 0 \\
c(t,0) & = & c_b(t) \in [0,1], \quad t > 0 \\
u(t,0) & = & u_b(t) > 0, \quad t > 0
\end{array}
\right.
$$

The 2×2 system

We analyse the system in terms of hyperbolicity system of P.D.E provided we exchange the time and space variables :

x is the evolutive variable, not t

$$\left\{ \begin{array}{rcl} \partial_x(u\,c) + \partial_t(c + q_1(c)) & = & 0 \\ \partial_x u + \partial_t h(c) & = & 0 \end{array} \right.$$

with conservative quantities

$$\boldsymbol{m = u\,c}, \qquad \boldsymbol{u} = u\,\rho$$

m is the flow rate of the first species
$u\rho$ is the total flow rate

Hyperbolicity

$$\text{Eigenvalues : } \mathbf{0} \text{ and } \boldsymbol{\lambda} = \frac{\boldsymbol{H(c)}}{\boldsymbol{u}}$$

$$\text{with } H(c) = 1 + (1-c)\, q_1' - c\, q_2' \geq 1$$

If $u > 0$, the system is strictly hyperbolic. Moreover :

$$d\lambda \cdot r = \frac{H(c)}{u^2}\, f''(c)$$

with r the associated eigenvector to λ and

$$\mathbf{f}(\mathbf{c}) = q_1(c) - c\, h(c) = (1-c)q_1(c) - cq_2(c)$$

λ is genuinely nonlinear if *f"* $\neq$ 0

Examples

Langmuir isotherm :

$$q_1(c) = \frac{Q_1\, K_1\, c}{1 + K_1\, c + K_2\,(1-c)}, \quad q_2(c) = \frac{Q_2\, K_2\,(1-c)}{1 + K_1\, c + K_2\,(1-c)}$$

$\mathbf{f}''$ keeps a constant sign

BET isotherm : with an inert gas ($q_2(c) = 0$) and

$$q_1(c) = \frac{Q\, K\, c}{(1 + Kc - (c/c_s))(1 - (c/c_s))}, \quad Q > 0,\ K > 0,\ c_s > 0,$$

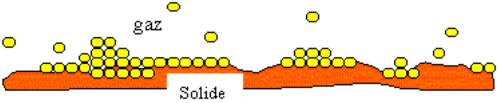
then $\mathbf{f}(\mathbf{c}) = (\mathbf{1} - \mathbf{c})\,\mathbf{q_1}(\mathbf{c})$ is not concave and not convex

Remarks

Generally, isotherms are not convex except some important cases (Langmuir, ammoniac, water vapour)

Interpretation :

at each inflexion point a new layer starts on the pervious layer



Riemann Invariants

For smooth solutions

$$\partial_x \left(u\, G(c) \right) = 0$$

$$\partial_x c + \frac{H(c)}{u}\, \partial_t c = 0$$

with

$$g' = \frac{-h'}{H},\; G = \exp(g)$$

There are two Riemann invariants :

$$c \quad \text{and} \quad W = u\, G(c) = u\, e^{g(c)}$$

Entropies

Entropies :

$$\boldsymbol{S(c,u) = \phi(uG(c)) + u\,\psi(c)}$$

where ϕ and ψ are smooth functions

Entropy-flux $Q = Q(c)$ satisfies

$$\boldsymbol{Q'(c) = h'(c)\,\psi(c) + H(c)\,\psi'(c)}$$

$$\Rightarrow \partial_t S + \partial_x Q = 0$$

Convex entropy ?

For any convex function ψ,

$$\boldsymbol{S_2(c,u) = u\,\psi(c)}$$

is convex (but not strictly convex)

There are strictly convex entropies of the form

$$S_1(c,u) = \phi(uG(c)) \Leftrightarrow$$

$$G'' = (g'' + g'^2)\exp(g) \neq 0 \text{ for } c \in [0,1]$$

Weak entropy solutions

Definition

Let $T > 0$, $X > 0$,

$$u \in L^\infty((0,T) \times (0,X)) \text{ and } 0 \leq c(t,x) \leq 1 \text{ p.p. in } (0,T) \times (0,X)$$

then (c, u) is a weak entropy solution if for any convex function ψ :

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

with $Q' = H\psi' + h'\psi$

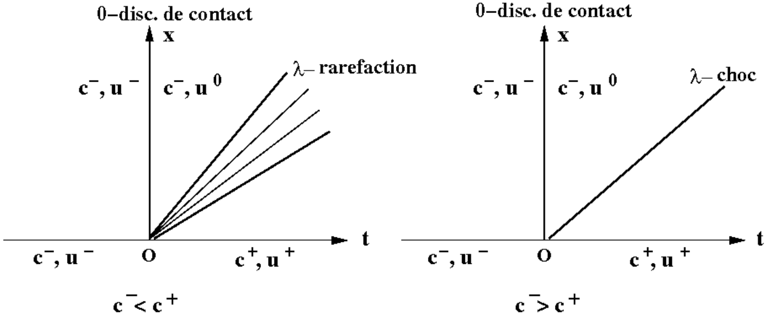
Remark : if $\pm G'' > 0$ on $[0,1]$, we also have :

$$\pm\,\boldsymbol{\partial_x\,(u\,G(c)) \leq 0}, \text{ on } \mathbf{[0,1]}$$

Riemann problem

Rappel : c is a Riemann invariant

If f is convex :



through a λ-wave $TV[\ln(u(z))] \leq \gamma\,|c^+ - c^0|, z = \dfrac{x}{t}$

Contents

Godunov scheme

The convergence of the Godunov scheme is generally an open problem for a 2×2 system

- LeVeque, Randall J. ; Temple, Blake, 1985
  Stability of Godunov's method for a class of 2×2 systems of conservation laws
  Trans. Amer. Math. Soc. 288
- Bressan, Alberto ; Jenssen, Helge Kristian, 2001
  Convergence of the Godunov scheme for straight line systems
- Bressan, Alberto ; Jenssen, Helge Kristian ; Baiti, Paolo, 2006
  An instability of the Godunov scheme
  Comm. Pure Appl. Math. 59

An existence result

Let be $X > 0$, $T > 0$. We assume :

$$c_0 \in BV(0,X), c_b \in BV(0,T), u_b \in L^\infty(0,T)$$

$$0 \leq c_0,\ c_b \leq 1 \quad \text{and} \quad \inf_{0<t<T} u_b(t) > 0$$

Then there exists an entropy solution (c, u) such that :

$$0 \leq \min(\inf c_b, \inf c_0) \leq c \leq \max(\sup c_b, \sup c_0) \leq 1$$
$$|u| \leq \|u_b\|_\infty \exp(\gamma\, TV(c_l)) \quad \text{and} \quad \inf u > 0$$
$$c \in L^\infty((0,T); BV(0,X)) \cap L^\infty((0,X); BV(0,T))$$
$$\ln(u) \in L^\infty((0,T); BV(0,X))$$

Front Tracking Algorithm (FTA)

With the assumption :

the eigenvalue λ is genuinely non linear

this scheme shows again the existence of an entropy solution but more precisely the specific structure of the velocity in two cases :

- the case with smooth concentrations
- the more complicated case with BV concentrations

$$u_b \in BV[0,T] \Rightarrow u \in BV([0,T] \times [0,X])$$

not given by the Godunov scheme !

A. Corli and O. Gues, Stratified solutions for systems of conservation laws, Trans. Amer. Math. Soc., 2001

Front Tracking Algorithm (FTA)

The stratified specific structure of the velocity $L_t^\infty \times BV_{t,x}$

$$u(t,x) = u_b(t)v(t,x)$$

has interesting applications

- the stability in strong topologies of concentrations with respect to weak* limits for the incoming velocity
- an example of blow-up

but there is an assumption $f" > 0$ and then the eigenvalue λ is genuinely non linear

Contents

“Blow up” with L^∞ data

Examples for $N \times N$ hyperbolic systems

- with $N \geq 3$
  - Helge Kristian Jenssen ; Carlo Sinestrari. CPDE (1999)
  - Helge Kristian Jenssen ; Robin Young. JHPDE (2004)
  - Michael, Sever
    Distribution solutions of nonlinear systems of conservation laws
    Mem. Amer. Math. Soc. 190 (2007),
- with $N = 2$
  - Robin Young : SIMA 99, CM 03, CMS 03

    2 Burgers equations linearly coupled at 2 boundaries
  - Bourdarias, Gisclon, Junca, JHPDE (2010).
    Blow up for a 2×2 chemical system with 1 characteristic boundary

Entropy and Riemann invariant $W = uG(c) \nearrow$

- Maximum Principle for $c(t,x) : 0 \leq c \leq 1$ but not for $u(t,x)$!

$$u \to +\infty$$

- $G'' < 0 \Rightarrow \partial_x(uG(c)) \geq 0$

- avoid Temple system
  - Temple, Blake, Trans. Amer. Math. Soc. (1983)
  - Bressan, Alberto ; Goatin, Paola
    Stability of L^∞ solutions of Temple class systems
    Differential Integral Equations 13 (2000)
  - Bianchini, Stefano
    Stability of L^∞ solutions for hyperbolic systems with coinciding shocks and rarefactions
    SIAM J. Math. Anal. 33 (2001)

Temple system ?

Generally, it is not a Temple system (ammonia, water vapor)

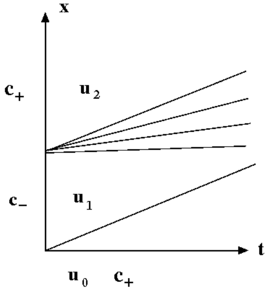
If $f'' > 0$, it is a Temple system iff

$$\partial_x(uG(c)) = 0$$

Examples :

If $G'' \equiv 0$ (for example two linear isotherms) then it is a Temple system
If $q_1 \equiv 0$ (gas 1 inert), it is a Temple system iff $q_2'' \equiv 0$

Brick for the blow up



We assume that the system is not a Temple system, that

$$f'' < 0 \text{ and } h' < 0 \text{ (no restrictive)}$$

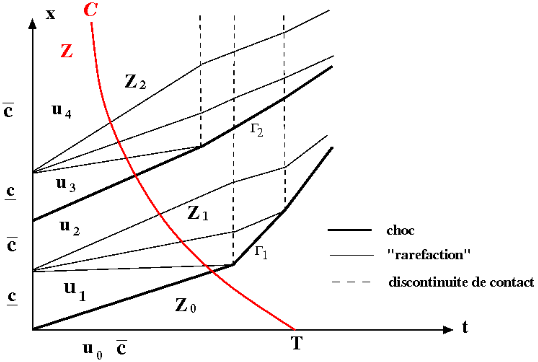
then there exists a choice of $c_- < c_+$ such that

$$u_2 = \mathbf{R}(c_-, c_+)u_0$$

with

$$G'' < 0 \Rightarrow W = uG(c) \nearrow \quad \Rightarrow \quad \mathbf{R}(c_-, c_+) \geq 1$$

Iterations



- $\forall (c_-, c_+) \quad R(c_-, c_+) = 1 \Leftrightarrow$ the system is in the Temple class
- if the system is not a Temple system then

$$\exists c_- < c_+, \qquad \mathbf{R}(c_-, c_+) > 1$$

Unique Solution with the Front Tracking Algorithm

Blow up at $X > 0$

- In Z, explicit solution before interactions
- Interactions outside Z
- Unique piecewise smooth solution on $[0, X - \varepsilon] \times \mathbb{R}$, $\varepsilon > 0$
  Bourdarias, Gisclon, Junca : JMAA 06
- $u(0, X) = +\infty$
- The boundary becomes twice characteristic : $\lambda = 0$
- $TVc_0 = TVc(t = 0, [0, X]) = +\infty$

An example of “Blow up”

Blow-up

Under the assumptions :

- $\boldsymbol{G'' < 0}$
- h' et f'' do not vanish
- the system is not a Temple system

we can construct an solution such that $\forall T > 0$, $\forall X > 0$, when $x \to X$

$\| u(.,x) \|_{L^\infty(0,T)} \to +\infty$, $\lambda = \dfrac{H(c)}{u} \to 0$, c stays bounded

Remarks :

- $G'' < 0 \Rightarrow \partial_x(uG(c)) \geq 0$: $-uG(c)$ is a convex entropy
- $h' \neq 0 \Rightarrow$ one gas is more active than an another
- $f'' \neq 0 \Rightarrow$ the eigenvalue λ is genuinely non linear

Chemical Examples : ammoniac, water vapor

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Prospects and open problems

- Existence of solution on $[0, X = +\infty[$ with
$$u(0, x) = +\infty \text{ for } x \geq X?$$
(proof tentative : problem with the O-waves)
- Validity of the model
- Relaxation
- Theory L^∞ with some restrictions on the data admissible initial boundary value data $u_b, c_b, c_0 \in L^\infty$
$$\text{such that } u(0, X) < +\infty$$
- Existence in fractional BV spaces : BV^s, $0 < s < 1$ with
$$u_b \in L^\infty \text{ and } c_0, c_b \in BV^{1/2 \text{ or } 1/3}$$
- Kinetic problem
- Nonisothermal model

Contents

C. Bourdarias, M. Gisclon and S. Junca

- *Some mathematical results on a system of transport equations with an algebraic constraint describing fixed-bed adsorption of gases*. J. Math. Anal. Appl., 2006
- *Existence of Weak Entropy Solutions for Gas Chromatography system with one or two active species and non Convex Isotherms*. Commun. Math. Sci., 2007
- *Hyperbolic models in gas-solid chromatography*
  Bol. Esp. Mat. Apl., 2008
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- *Blow up at the hyperbolic boundary for a 2×2 system arising from chemical engineering*. J. Hyperbolic Differ. Equ., 2010
- *BV^s spaces and applications to scalar conservation laws*
- *A kinetic scheme for a hyperbolic system arising in gas chromatography*