

A converging entropy scheme for one dimensional non-zero flux cross diffusion system

PODVIN Nicolas

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Introduction

The aim of this paper is to introduce a numerical scheme for a one-dimensional cross-diffusion equation with non-zero fluxes. These equations models a variety of phenomena and their studies are motivated by their application to Physical Vapour Deposition (PVD), involved in the fabrication of solar panel cells.

To produce those cells, a wafer is introduced into a hot chamber along with several chemicals under gaseous forms. Those gases are depositing a substrate onto the wafer, allowing the formation of a thin heterogeneous solid. While the wafer is in the chamber, two main phenomena has to be accounted for: the deposition of the gases onto the wafer and the diffusion of the many different species onto the thin solid.

We chose to model a one-dimensional solid, where the deposition from the gases are modelled by chemical fluxes arriving at one extremity. We assume that the process occurs during times $t \in (0, T)$ for a given finite horizon $T > 0$. Let us say that there is $N \in \mathbb{N}^*$ chemical species and the flux for specie $i \in \{1, \dots, N\}$ is denoted $\phi_i \in L^\infty(\mathbb{R}^+, \mathbb{R}^+)$. Figure 1 illustrate such model :

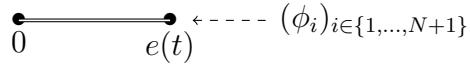


Figure 1: One dimensional model: $e(t)$ is the thickness of the domain at time t (changing through time)

This paper follows the physical model described in [1], recalled in Section 1. After presenting the discretization in Section 2, the numerical scheme is defined in Section 3, inspired by [2], as well as a number of key properties such as the stability of a set \mathcal{A} transcribing the physical property of concentrations, and an entropy decay. Section 4 present compactness results for the discrete solution, which are in turn used to prove the convergence of the scheme in section 5. We also studied the case of constant fluxes in section 6 which yields a predictable long-term behavior as shown in [1] which is preserved in our scheme. Numerical simulation are illustrated in Section 7 for a piece-wise constant flux setting, and in Section 8 for the case of constant flux echoing Section 6.

1 Continuous Setting

1.1 Evolution problem

We will follow the model described in [1]. Firstly, we assume that the fluxes $(\phi_i)_i$ are known, that is, from the two main phenomena described above, we wish to study the diffusion of all species inside the thin solid given the deposition from the gases. We assume that the solid starts with a thickness $e_0 \in \mathbb{R}_+^*$ and that the evolution of the thickness is:

$$\forall t \in (0, T) \quad e(t) = e_0 + \int_0^t \sum_{i=1}^N \phi_i(s) ds.$$

Let us call $(u_i(t, x))_i$ the normalized concentration of the specie i at time $t \in (0, T)$ on the location $x \in (0, e(t))$ and defining the symmetric matrix $(a_{ij})_{i,j \in \{1, \dots, N\}}$ representing diffusion from specie i to specie j . The cross-diffusion evolution can be written as :

$$\partial_t u_i = \partial_x \left[\sum_{j=1}^N a_{ij} (u_j \partial_x u_i - u_i \partial_x u_j) \right] \quad \text{on } (0, T) \times (0, e(t)).$$

Let us mention right away that the notation " $(0, T) \times (0, e(t))$ " is explicit but ambiguous w.r.t. the variable t . Though we will keep using it, a more rigorous definition would be :

$$Q_T := \bigcup_{t \in (0, T)} \{t\} \times (0, e(t)).$$

As u_i represent a concentration (up to renormalization), it is natural to impose that the concetration vector $\underline{u} := [u_1 \dots u_N]^T$ belongs to the space :

$$\mathcal{A} = \left\{ U \in \mathbb{R}_+^N , \sum_i u_i = 1 \right\},$$

and a vectorized version of the evolution can be written as

$$\partial_t \underline{u} = \partial_x \left[A(\underline{u}) \partial_x \underline{u} \right] \quad \text{on } (0, T) \times (0, e(t))$$

for a fixed matrix $A(\underline{u})$. Regarding the boundary conditions, we assume no flux occurs at $x = 0$. From the analysis of the cross-diffusion matrix (see for instance [3]), we can show that the matrix $A(\underline{u})$ is non-singular, given that \underline{u} belongs to \mathcal{A} . Therefore this no-flux boundary condition is equivalent to :

$$\sum_{j=1}^N a_{ij} (u_j(t, 0) \partial_x u_i(t, 0) - u_i(t, 0) \partial_x u_j(t, 0)) = 0.$$

To determine the boundary condition at $x = e(t)$, we assume the following mass conservation law applies for each specie :

$$\forall t \in (0, T) \quad \frac{d}{dt} \left(\int_0^{e(t)} u_i(t, x) dx \right) = \phi_i(t),$$

yielding:

$$\forall t \in (0, T) \quad \sum_{j=1}^N a_{ij}(u_j(t, 1) \partial_x u_i(t, 1) - u_j(t, 1) \partial_x u_i(t, 1)) + e'(t) u_i(t, e(t)) = \phi_i(t).$$

At this point, given an initial profile (i.e. set of N -initial concentration) in \mathcal{A} , we have a problem with initial condition, boundary conditions at every point of the frontier of our domain and an evolution equation. But to ensure its well-posedness, having a *moving-in-time* domain raises issues. We therefore introduce the following change of variables by defining for a specie i :

$$v_i : (0, T) \times (0, 1) \quad (t, x) \mapsto u_i(t, e(t)x).$$

From this change of variable, we have the following problem :

$$\left\{ \begin{array}{l} \text{Find } (v_1, \dots, v_N) \text{ such that :} \\ \\ e(t) = e_0 + \int_0^t \sum_{i=1}^N \phi_i(s) ds \\ \\ \partial_t v_i = e^{-2}(t) \partial_x \left[\sum_{j=1}^N a_{ij} (v_j \partial_x v_i - v_i \partial_x v_j) \right] + x \partial_x v_i \quad \forall i \in 1, \dots, N \text{ on } (0, T) \times (0, 1) \\ \\ \sum_{j=1}^N a_{ij} (v_j \partial_x v_i - v_i \partial_x v_j)(t, 0) = 0 \\ \\ \sum_{j=1}^N a_{ij} (v_j \partial_x v_i - v_i \partial_x v_j)(t, 1) = e(t) e'(t) \left(\frac{\phi_i(t)}{e'(t)} - v_i(t, 1) \right), \end{array} \right.$$

with initial conditions $(v_1, \dots, v_N) \in L^\infty((0, T) \times (0, 1), \mathcal{A})$. A solution of the previous problem shall be denoted as *strong solution*.

We can see from above that this shift in perspective allowed us to set a fixed domain, but added a *drift term* to account for the relative displacement of concentrations.

1.2 Weak formulation

We shall study an approximation of the strong solution by using *weak formulation*. Taking $\psi \in \mathcal{C}_c^1([0, T] \times [0, 1])$ and defining $Q_T = (0, T) \times (0, 1)$, it holds:

$$\iint_{Q_T} v_i \partial_t \psi + \int_0^1 v_i^0 \psi(0) = \iint_{Q_T} \frac{1}{e^2(t)} \partial_x \psi \sum_{j=1}^N a_{ij} (v_j \partial_x v_i - v_i \partial_x v_j) + \iint_{Q_T} \frac{e'}{e} v(x \partial_x \psi + \psi) - \int_0^T \frac{\phi_i}{e} \psi(., 1). \quad (1)$$

A solution to Equation (1) is referred as a *weak solution*, and shall be the target for our discrete model in the sense that the discretization will aim to converge to Equation (1).

2 Discrete settings

2.1 Time discretization

For the time discretization, we use a standard piecewise constant discretization induced by a grid of the interval $[0, T]$ into *regular* subintervals $([t_{n-1}, t_n])_{n \in [|1, N_T|]}$ for a given integer N_T with Δt the size of each subinterval. We therefore shall denote the piecewise constant approximation for a temporal function $f : [0, T] \mapsto \mathbb{R}$:

$$\forall n \in [|1, N_T|] \quad f^n := \sum_{n=1}^{N_T} f(t) \mathbf{1}_{t \in [t_{n-1}, t_n]},$$

with $\mathbf{1}$ being the notation used for the indicator function.

2.2 Space discretization

Due to the nature of our problem ,we chose to use a Finite Volume scheme. In our one-dimension problem, this amounts to dividing $(0, 1)$ into N_d intervals (sometimes denoted as "cell", analogous to a higher dimension discretization) of size Δx with centers $(x_k)_{k \in [|1, N_d|]}$. Since we are using a Finite Volume scheme, our approximation of the problem will require to also evaluate values at the edges of our intervals, denoted $(x_{k+\frac{1}{2}})_{k \in [|0, N_d|]}$.

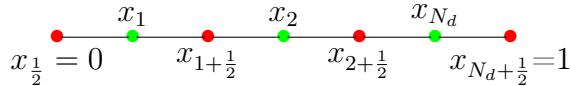


Figure 2: Spatial discretization ($N_d = 3$)

where we have according to Figure 2:

$$\begin{cases} \forall k \in [|1, N_d|] & x_k = \left(k + \frac{1}{2}\right) \Delta x, \\ \forall k \in [|1, N_d|] & x_{k-\frac{1}{2}} = (k - 1) \Delta x, \\ \forall k \in [|0, N_d|] & x_{k+\frac{1}{2}} = k \Delta x. \end{cases}$$

To keep the number of unknown to be N_d , we approximate those edge values using the cell center values, in two distinct ways. First, the logarithmic mean approach, setting for each i :

$$\forall k \in [|1, N_d - 1|] \quad v_{i,k+\frac{1}{2}} = \begin{cases} 0 & \text{if } \min(v_{i,k}, v_{i,k+1}) \leq 0 \\ v_{i,k} & \text{if } v_{i,k} = v_{i,k+1} \\ \frac{v_{i,k+1} - v_{i,k}}{\ln(v_{i,k+1}) - \ln(v_{i,k})} & \text{otherwise,} \end{cases} \quad (2)$$

and the normalized log-mean approach :

$$\forall k \in [|1, N_d - 1|] \tilde{v}_{i,k+\frac{1}{2}} = \frac{v_{i,k+\frac{1}{2}}^n}{\sum_{j=1}^N v_{j,k+\frac{1}{2}}^n}, \quad (3)$$

while $(v_{i,\frac{1}{2}}, v_{i,N_d+\frac{1}{2}})$ are determined according to the boundary conditions.

The choice of the previous approximation (using an inverted log-mean) will become clear once we introduce *discrete Entropy* estimates (this will allow a discrete logarithmic chain rule to apply), whereas the normalization described in 3 will ensure stability for the sum over all species.

We define the discrete derivative as centered on $k \in \{1, \dots, N_d - 1\}$, upward for $k = 0$ and downward for $k = N_d$:

$$D_{k+\frac{1}{2}}(c) = \begin{cases} \frac{2(c_1 - c_{1+1/2})}{\Delta x} & \text{if } k = 0 \\ \frac{2(c_{N_d+1/2} - c_{N_d})}{\Delta x} & \text{if } k = N_d \\ \frac{c_{k+1} - c_k}{\Delta x} & \text{otherwise.} \end{cases} \quad (4)$$

2.3 Entropy

We define here the *discrete Entropy*, analogous to the continuous' found in [1] Anticipating the scheme stability w.r.t \mathcal{A} , setting $\Omega = (0, 1)$:

$$\forall n \in [|0, N_T|] \quad E^n = \sum_{k=1}^{N_d} \sum_{i=1}^N \Delta x v_{i,k}^n \ln(v_{i,k}^n).$$

In addition, if it holds that $v_{i,k} \in (0, 1)$ for all couple $(i, k) \in [|1, N|] \times [|1, N_d|]$, then by noting that $x \mapsto x \ln x$ maps $(0, 1)$ into $(-\frac{1}{e}, 0)$ and that $\sum_{k=1}^{N_d} \Delta x = 1$, we have the bounds for the entropy :

$$\forall n \in [|0, N_T|] \quad E^n \in \left[-\frac{N}{e}, 0 \right].$$

3 Numerical Scheme - Properties

3.1 Conservation Law

Given a cell $k \in [|1, \dots, N_d|]$, the following Implicit Euler scheme holds for all time step n and specie i :

$$T_{time} = T_{diff,a^*} + T_{diff,a_{ij}} + T_{drift},$$

where :

$$T_{time} = \Delta x \frac{v_{i,k}^n - v_{i,k}^{n-1}}{\Delta t}, \quad (5)$$

$$T_{diff,a^*} = \frac{a^*}{(e^n)^2} \left[D_{k+\frac{1}{2}}(v_i^n) - D_{k-\frac{1}{2}}(v_i^n) \right], \quad (6)$$

$$T_{diff,a_{ij}} = \frac{1}{(e^n)^2} \left[\sum_{j=1}^N (a_{ij} - a^*) \left(v_{j,k+\frac{1}{2}}^n D_{k+\frac{1}{2}}(v_i^n) - v_{j,k-\frac{1}{2}}^n D_{k-\frac{1}{2}}(v_i^n) \right) \right] \quad (7)$$

$$- \sum_{j=1}^N (a_{ij} - a^*) \left(v_{i,k+\frac{1}{2}}^n D_{k+\frac{1}{2}}(v_j^n) - v_{i,k-\frac{1}{2}}^n D_{k-\frac{1}{2}}(v_j^n) \right), \quad (8)$$

$$T_{drift} = \frac{(e')^n}{e^n} \left[(x_{k+\frac{1}{2}} \tilde{v}_{i,k+\frac{1}{2}}^n - x_{k-\frac{1}{2}} \tilde{v}_{i,k-\frac{1}{2}}^n) - \Delta x v_{i,k}^{n-1} \right]. \quad (9)$$

Where we defined :

$$\begin{cases} e^0 = e_0 \\ e^n = e^{n-1} + \Delta t (e')^n \\ (e')^n = \sum_{j=1}^N \phi_j^n. \end{cases} \quad (10)$$

This is a classical Euler Implicit scheme, except for a part of the drift term which is expressed explicitly. This allows to adapt the mass conservation at a discrete level.

3.2 Boundary Conditions

Let us set $n \in \llbracket 1, N_T \rrbracket$. For the left BC, at $x = 0$, it can be shown (c.f. [3]) that it is equivalent to a no flux BC, therefore :

$$\forall i \in \llbracket 1, N \rrbracket \quad D_{\frac{1}{2}}(v_i^n) = 0.$$

Regarding the BC at $x = 1$, the discrete BC yields :

$$\sum_{j=1}^N a_{ij} \left(v_{j,N_d+\frac{1}{2}}^n D_{N_d+\frac{1}{2}}(v_i^n) - v_{i,N_d+\frac{1}{2}}^n D_{N_d+\frac{1}{2}}(v_j^n) \right) = e^n (e')^n \left[\frac{\phi_i^n}{(e')^n} - v_{i,N_d+\frac{1}{2}}^n \right].$$

Noting that $(e')^n = \sum_{i=1}^N \phi_i^n$, and using the symmetry of (a_{ij}) , by summing over i , we can show that :

$$\sum_{i=1}^N v_{i,N_d+\frac{1}{2}}^n = 1.$$

For the right BC at $x = 1$, writing :

$$\forall i \in \llbracket 1, N \rrbracket \quad \sum_{j=1}^N a_{ij} \left(v_{j,N_d+\frac{1}{2}}^n D_{N_d+\frac{1}{2}}(v_i^n) - v_{i,N_d+\frac{1}{2}}^n D_{N_d+\frac{1}{2}}(v_j^n) \right) = (e')^n e^n \left[\frac{\phi_i^n}{(e')^n} - v_{i,N_d+\frac{1}{2}}^n \right],$$

we can see that the N -dimensionnal vector $\underline{V}_{N_d+\frac{1}{2}}^n = (v_{j,N_d+\frac{1}{2}}^n)_j$ can be expressed as the solution of the linear problem :

$$\underline{\underline{B}}(V_{N_d}^n)V_{N_d+\frac{1}{2}}^n = e^n \underline{\phi}^n, \quad (11)$$

where :

$$\begin{cases} [\underline{\underline{B}}]_{ii} = (e')^n e^n + \frac{2}{h} \sum_{j \neq i} a_{ij} v_{j,N_d}, \\ [\underline{\underline{B}}]_{i \neq j} = -\frac{2}{h} a_{ij} v_{i,N_d}. \end{cases}$$

3.3 Mass Conservation

We sum all contributions for all cells $k \in [|1, \dots, N_d|]$ to illustrate the mass conservation. Let us show on all contributions :

$$\begin{aligned} T_{time} &= \sum_{k=1}^{N_d} \Delta x (\Delta t)^{-1} v_{i,k}^n - \sum_{k=1}^{N_d} \Delta x (\Delta t)^{-1} v_{i,k}^{n-1}, \\ T_{diff,a^*} &= \frac{a^*}{(e^n)^2} \left[D_{N_d+\frac{1}{2}}(v_i^n) - D_{\frac{1}{2}}(v_i^n) \right] = \frac{a^*}{(e^n)^2} D_{N_d+\frac{1}{2}}(v_i^n), \\ T_{diff,a_{ij}-a^*}^{a^*-term} &= -\frac{a^*}{(e^n)^2} \left[\left(D_{N_d+\frac{1}{2}}(v_i^n) \left(\sum_j v_{j,N_d+\frac{1}{2}} \right) - D_{\frac{1}{2}}(v_i^n) \left(\sum_j v_{j,\frac{1}{2}} \right) \right) \right. \\ &\quad \left. - \left(v_{i,N_d+\frac{1}{2}} \left(\sum_j D_{N_d+\frac{1}{2}}(v_j^n) \right) - v_{i,\frac{1}{2}} \left(\sum_j D_{\frac{1}{2}}(v_j^n) \right) \right) \right] \\ &= -\frac{a^*}{(e^n)^2} D_{N_d+\frac{1}{2}}(v_i^n), \\ T_{diff,a_{ij}-a^*}^{a_{ij}-term} &= \frac{(e')^n}{e^n} \left[\frac{\phi_i^n}{(e')^n} - v_{i,N_d+\frac{1}{2}}^n \right], \\ T_{drift} &= \frac{(e')^n}{e^n} \left[v_{i,N_d+\frac{1}{2}}^n - \sum_{k=1}^{N_d} \Delta x v_i^{n-1} \right]. \end{aligned}$$

Therefore the conservation equation becomes :

$$\sum_{k=1}^{N_d} \Delta x v_{i,k}^n = \sum_{k=1}^{N_d} \Delta x v_{i,k}^{n-1} + \Delta t \frac{(e')^n}{e^n} \left[\frac{\phi_i^n}{(e')^n} - \sum_{k=1}^{N_d} \Delta x v_{i,k}^{n-1} \right].$$

Multiplying by e^n and using (10) :

$$\begin{aligned} \sum_{k=1}^{N_d} e^n \Delta x v_{i,k}^n &= \sum_{k=1}^{N_d} e^{n-1} \Delta x v_{i,k}^{n-1} + \Delta t \sum_{k=1}^{N_d} (e')^n \Delta x v_{i,k}^{n-1} + \Delta t \left[\phi_i^n - \sum_{k=1}^{N_d} (e')^n \Delta x v_{i,k}^{n-1} \right] \\ &= \sum_{k=1}^{N_d} e^{n-1} \Delta x v_{i,k}^{n-1} + \Delta t \phi_i^n. \end{aligned}$$

Therefore :

$$\frac{\sum_{k=1}^{N_d} e^n \Delta x v_{i,k}^n - \sum_{k=1}^{N_d} e^{n-1} \Delta x v_{i,k}^{n-1}}{\Delta t} = \phi_i^n. \quad (12)$$

This mirror the mass conservation in the continuous setting, and keeping this conservation at the discrete level impose that a part of the drift term is being written in terms of $v_{i,k}^{n-1}$ instead of $v_{i,k}^n$.

3.4 Stability of \mathcal{A} : summation to 1

Let us assume that $\sum_{j=1}^N v_{j,k}^{n-1} = 1$ for a given integer $n \in \mathbb{N}^*$. The conservation laws yields for the sum over all species, denoting $S_k^n := \sum_{i=1}^N v_{i,k}^n$:

$$\begin{aligned}\Delta x(\Delta t)^{-1}(S_k^n - S_k^{n-1}) &= \frac{a^*}{(e^n)^2} \left[D_{k+\frac{1}{2}}(S^n) - D_{k-\frac{1}{2}}(S^n) \right] \\ &\quad + \frac{(e')^n}{e^n} \left((x_{k+\frac{1}{2}} - x_{k-\frac{1}{2}}) \times 1 - \Delta x S_k^{n-1} \right) \\ &= \frac{a^*}{(e^n)^2} \left[D_{k+\frac{1}{2}}(S^n) - D_{k-\frac{1}{2}}(S^n) \right].\end{aligned}$$

Denoting $\underline{S}^n \in \mathbb{R}^{N_d}$ the vector $(S_k^n)_k$ and $(e_k)_k$ the canonical basis of \mathbb{R}^{N_d} , we have the following system, writing $C_{x,t} := \frac{a^*}{e^n} \frac{dt}{dx^2}$:

$$(\underline{I}_{N_d} - C_{x,t} \underline{A}) \underline{S}^n = \underline{1} + 2C_{x,t} e_{N_d}.$$

An obvious solution to this equation is $\underline{S}^n = \underline{1}$, and to prove it is the only one, one needs to verify that the matrix $(\underline{I}_{N_d} - C_{x,t} \underline{A})$ is non-singular.

We can explicit the matrix :

$$\underline{I}_{N_d} - C_{x,t} \underline{A} = \begin{bmatrix} 1 + C_{x,t} & -C_{x,t} & 0 & 0 & 0 & \dots & 0 \\ -C_{x,t} & 1 + 2C_{x,t} & -C_{x,t} & 0 & 0 & \dots & 0 \\ 0 & -C_{x,t} & 1 + 2C_{x,t} & -C_{x,t} & 0 & \dots & 0 \\ \vdots & & \ddots & & & & \vdots \\ \vdots & & & \ddots & & & \vdots \\ 0 & & & & -C_{x,t} & 1 + 2C_{x,t} & -C_{x,t} \\ 0 & & \dots & & 0 & -C_{x,t} & 1 + 3C_{x,t} \end{bmatrix}$$

A sufficient condition to ensure non-singularity is obtained if the previous matrix is an M -matrix, which is obtained for any couple $(\Delta x, \Delta t) \in (\mathbb{R}^+)^2$.

3.5 Stability of \mathcal{A} : nonnegativity

The proof relies on assuming $\min_{i,k} v_{i,k}^n < 0$ and arriving to a contradiction.

We observe that with v_{i_0,k_0} being the min, we get :

- $D_{k+\frac{1}{2}}(v_{i_0}^n) \geq 0$, for $k \in [|1, N_d - 1|]$
- $D_{k-\frac{1}{2}}(v_{i_0}^n) \leq 0$, for $k \in [|1, N_d|]$
- $v_{i_0,k-\frac{1}{2}} = 0$, for $k \in [|1, N_d|]$ and $v_{i_0,k+\frac{1}{2}} = 0$, for $k \in [|1, N_d - 1|]$
- $\tilde{v}_{i_0,k-\frac{1}{2}} = 0$, for $k \in [|1, N_d|]$ and $\tilde{v}_{i_0,k+\frac{1}{2}} = 0$, for $k \in [|1, N_d - 1|]$.

Noting that

$$T_{time} = \Delta x(\Delta t)^{-1}(v_{i_0,k_0}^n - v_{i_0,k_0}^{n-1}) \leq 0,$$

which yields :

$$T_{diff,a^*} + T_{diff,ij} + T_{drift} \leq 0.$$

For $k_0 \in [|1, N_d - 1|]$

The a^* -terms yields :

$$\frac{a^*}{e^2(t)} \left[D_{k_0+\frac{1}{2}}(v_{i_0}^n) \left(1 - \sum_j v_{j,k_0+\frac{1}{2}} \right) - D_{k_0-\frac{1}{2}}(v_{i_0}^n) \left(1 - \sum_j v_{j,k_0-\frac{1}{2}} \right) \right],$$

which is nonnegative due to the definitions of the half terms (the ln-mean is lower than arithmetic mean, this by a trapeze rule over the exponential).

The remaining a_{ij} -term yields the following nonnegative quantity:

$$T_{diff,a_{ij}-a^*}^{a_{ij}term} = \frac{1}{(e^n)^2} \left[D_{k_0+\frac{1}{2}}(v_{i_0}^n) \sum_j (a_{ij} v_{j,k_0+\frac{1}{2}}^n) - D_{k_0-\frac{1}{2}}(v_{i_0}^n) \sum_j (a_{ij} v_{j,k_0-\frac{1}{2}}^n) \right].$$

Only the drift term remains:

$$\begin{aligned} T_{drift} &= \frac{(e')^n}{e^n} \left[x_{k_0+\frac{1}{2}} \tilde{v}_{i_0,k_0+\frac{1}{2}} - x_{k_0-\frac{1}{2}} \tilde{v}_{i_0,k_0-\frac{1}{2}} - \Delta x v_{i_0,k_0}^{n-1} - \Delta x v_{i_0,k_0}^n + \Delta x v_{i_0,k_0}^n \right] \\ &= -\frac{(e')^n}{e^n} \Delta x v_{i_0,k_0}^n + \frac{(e')^n}{e^n} \Delta x (v_{i_0,k_0+\frac{1}{2}}^n - v_{i_0,k_0-\frac{1}{2}}^{n-1}). \end{aligned}$$

The first part is nonnegative by assumption. The second part is placed into the T_{time} term :

$$T_{time}^{corr} := T_{time} - T_{drift}^{corr} = \Delta x \left[\frac{1}{\Delta t} - \frac{(e')^n}{e^n} \right] (v_{i_0,k_0+\frac{1}{2}}^n - v_{i_0,k_0+\frac{1}{2}}^{n-1}).$$

However, as we have :

$$\frac{1}{\Delta t} - \frac{(e')^n}{e^n} \geq 0 \Leftrightarrow \frac{\Delta t(e')^n}{e^{n-1} + \Delta t(e')^n} \leq 1,$$

the term $T_{time} - T_{drift}^{corr}$ is still nonpositive, which is not possible if $\min_{i,k} v_{i,k}^n < 0$, yielding the contradiction for this case.

The only remaining case to study is $k_0 = N_d$.

For all a^* dependant terms :

$$-\frac{a^*}{e^2(t)} D_{N_d-\frac{1}{2}} \left(1 - \sum_j v_{j,k_0-\frac{1}{2}} \right) \geq 0,$$

and due to the right BC, the other terms yield :

$$\frac{\phi_i}{e^n} - \frac{(e')^n}{e^n} \Delta x v_{i_0,N_d}^n,$$

which yields the same contradiction as previously.

Therefore, we have shown that a nonnegative solution at step $n-1$ stays nonnegative at the next step, for all time steps $n \in [|1, N_T|]$.

3.6 Positivity

Starting with $\int_0^1 v_i^0 > 0$, we can follow the same proof as before to show that a positive solution stays positive as well.

We therefore wish to show that if the previous solution $(v_{i,k}^{n-1})_{i,k}$ is positive, then the next solution of the scheme $(v_{i,k}^n)_{i,k}$ is positive as well.

Let us assume that the latter is nonpositive. As we already established that it must be nonnegative, and as the mass is increasing, starting from a vector v^0 such that its mass $\int_0^1 v_i^0$ is positive, we cannot have a solution where all cell-values $(v_{i,k}^n)_k$ are null.

This implies the following :

$$\exists (i_0, k_0) \in [|1, N|] \times [|1, N_d|] \quad (v_{i_0, k_0}^n = 0 \text{ and } v_{i_0, k_0+1}^n > 0) \text{ or } (v_{i_0, k_0}^n = 0 \text{ and } v_{i_0, k_0-1}^n > 0).$$

Let us first note that if $k_0 = N_d$, we would have from the linear system (11) :

$$\forall i \in [|1, N|] \quad \left(\sum_{j \neq i} \phi_j \right) v_{i, N_d + \frac{1}{2}} = 0,$$

which would imply that $v_{i, N_d + \frac{1}{2}} = 0$ for all species $i \in [|1, N|]$. Similarly, $k_0 = 1$ would also yield the left border value $v_{i, \frac{1}{2}}$ to be zero as well.

These observations implies that border terms will not have an effect on the computations.

We therefore have :

$$T_{time}^{corr} = \Delta x \left[\frac{1}{\Delta t} - \frac{(e')^n}{e^n} \right] (v_{i_0, k_0 + \frac{1}{2}}^n - v_{i_0, k_0 + \frac{1}{2}}^{n-1}) < 0.$$

This means that $T_{diff, a^*} + T_{diff, a_{ij}} + T_{drift} < 0$ for the cell k_0 regarding the specie i_0 (note that we chose this time to group the contributions according to a^* and $(a_{ij})_{i,j}$ this time).

The a^* -terms yields, after ridding ourselves of the terms $v_{i_0, k_0 \pm \frac{1}{2}}$ which are null :

$$\begin{aligned} T_{diff, a^*} &= \frac{a^*}{e^2(t)} \left[D_{k_0 + \frac{1}{2}}(v_{i_0}) \left(1 - \sum_{j=1}^N v_{j, k_0 + \frac{1}{2}} \right) - D_{k_0 - \frac{1}{2}}(v_{i_0}) \left(1 - \sum_{j=1}^N v_{j, k_0 - \frac{1}{2}} \right) \right]. \\ &\geq 0 \end{aligned}$$

The a_{ij} -term :

$$\begin{aligned} T_{diff, a_{ij}} &= \frac{1}{e^2(t)} \left[D_{k_0 + \frac{1}{2}}(v_{i_0}) \left(\sum_{j=1}^N a_{ij} v_{j, k_0 + \frac{1}{2}} \right) - D_{k_0 - \frac{1}{2}}(v_{i_0}) \left(\sum_{j=1}^N a_{ij} v_{j, k_0 - \frac{1}{2}} \right) \right] \\ &\geq 0, \end{aligned}$$

and the drift term is therefore equal to zero, becomes it only depends linearly on v_{i_0, k_0} and $v_{i_0, k_0 \pm \frac{1}{2}}$ (as the reader recalls that we corrected the semi-implicit $n-1$ term back into the temporal term).

We therefore have shown that there cannot be any (i_0, k_0) where the value of v^n vanishes, therefore the positivity of the scheme is guaranteed.

3.7 Entropy

Similarly as for the nonnegativity, we are going to write :

$$T_{drift} = \frac{(e')^n}{e^n} \left[x_{k+\frac{1}{2}} \tilde{v}_{i,k+\frac{1}{2}} - x_{k-\frac{1}{2}} \tilde{v}_{i,k-\frac{1}{2}} - \Delta x v_{i,k}^{n-1} - \Delta x v_{i,k}^n + \Delta x v_{i,k}^n \right].$$

And we are passing the $(n, n-1)$ error term into the temporal term :

$$\begin{aligned} T_{time}^{corr} &= \Delta x \left(\frac{1}{\Delta t} - \frac{(e')^n}{e^n} \right) (v_{i,k}^n - v_{i,k}^{n-1}), \\ T_{drift}^{corr} &:= \frac{(e')^n}{e^n} \left[x_{k+\frac{1}{2}} \tilde{v}_{i,k+\frac{1}{2}} - x_{k-\frac{1}{2}} \tilde{v}_{i,k-\frac{1}{2}} - \Delta x v_{i,k}^n \right]. \end{aligned}$$

This will allow us to express a non-increasing entropy scheme. Indeed, multiplying the conservation equation by $\Delta t ln(v_{i,k}^n)$ and summing over $(i, k) \in [|1, N|] \times [|1, N_d|]$ will yield an entropy inequality.

For the corrected temporal term after this operation, denoted $T_{time,ent}^{corr}$, by the convexity of $x \mapsto x \ln x$:

$$[\ln(v_{i,k}^n) + 1](v_{i,k}^n - v_{i,k}^{n-1}) \geq v_{i,k}^n \ln(v_{i,k}^n) - v_{i,k}^{n-1} \ln(v_{i,k}^{n-1}).$$

Multiplying by Δx then summing over (k, i) :

$$\sum_{i=1}^N \sum_{k=1}^{N_d} \Delta x \ln(v_{i,k}^n) (v_{i,k}^n - v_{i,k}^{n-1}) + \sum_{k=1}^{N_d} \Delta x \sum_{i=1}^N (v_{i,k}^n - v_{i,k}^{n-1}) \geq E^n - E^{n-1},$$

which yields in turn :

$$T_{time,ent}^{corr} \geq \left(1 - \frac{\Delta t (e')^n}{e^{n-1} + \Delta t (e')^n} \right) [E^n - E^{n-1}].$$

For the first a^* -term :

$$\begin{aligned} T_{diff,a^*,ent} &= \frac{a^*}{(e^n)^2} \Delta t \sum_{i=1}^N \left[\sum_{k=1}^{N_d} D_{k+\frac{1}{2}}(v_i^n) \ln(v_{i,k}^n) - \sum_{k=1}^{N_d} D_{k-\frac{1}{2}}(v_i^n) \ln(v_{i,k}^n) \right] \\ &= \frac{a^*}{(e^n)^2} \Delta t \sum_{i=1}^N \left[-\Delta x \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\ln(v_i^n)) + D_{N_d+\frac{1}{2}}(v_i^n) \ln(v_{i,N_d}^n) \right]. \end{aligned}$$

And :

$$\begin{aligned}
T_{diff,a_{ij}-a^*,ent}^{a^*term} &= -\Delta t \frac{a^*}{(e^n)^2} \sum_{i,j} \left[\sum_{k=1}^{N_d} v_{j,k+\frac{1}{2}} D_{k+\frac{1}{2}}(v_i^n) \ln(v_{i,k}^n) - \sum_{k=1}^{N_d} v_{j,k-\frac{1}{2}} D_{k-\frac{1}{2}}(v_i^n) \ln(v_{i,k}^n) \right. \\
&\quad \left. - \left(\sum_{k=1}^{N_d} v_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(v_j^n) \ln(v_{i,k}^n) - \sum_{k=1}^{N_d} v_{i,k-\frac{1}{2}} D_{k-\frac{1}{2}}(v_j^n) \ln(v_{i,k}^n) \right) \right] \\
&= -\Delta t \frac{a^*}{(e^n)^2} \sum_{i=1}^N \left[-\Delta x \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) \left[\sum_j v_{j,k+\frac{1}{2}} \right] D_{k+\frac{1}{2}}(\ln(v_i^n)) \right. \\
&\quad \left. + D_{N_d+\frac{1}{2}}(v_i^n) \left[\sum_j v_{j,N_d+\frac{1}{2}} \right] \ln(v_{i,N_d}^n) \right. \\
&\quad \left. - \left(-\Delta x \sum_{k=1}^{N_d-1} v_{i,k+\frac{1}{2}}^n D_{k+\frac{1}{2}}(\ln(v_i^n)) \left[\sum_j D_{k+\frac{1}{2}}(v_j^n) \right] + v_{i,k+\frac{1}{2}}^n \ln(v_{i,k}^n) \left[\sum_j D_{N_d+\frac{1}{2}}(v_j^n) \right] \right) \right].
\end{aligned}$$

Combinnig all a^* terms yields the following nonpositive term :

$$-\sum_{i=1}^N \sum_{k=1}^{N_d-1} v_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(v_i^n) \left(1 - \sum_{j=1}^N v_{j,k+\frac{1}{2}} \right) \leq 0.$$

For the a_{ij} -term :

$$\begin{aligned}
T_{diff,a_{ij}-a^*,ent}^{a_{ij}term} &= \Delta t \frac{1}{(e^n)^2} \sum_{i,j} a_{ij} \left[\sum_{k=1}^{N_d} v_{j,k+\frac{1}{2}} D_{k+\frac{1}{2}}(v_i^n) \ln(v_{i,k}^n) - \sum_{k=1}^{N_d} v_{j,k-\frac{1}{2}} D_{k-\frac{1}{2}}(v_i^n) \ln(v_{i,k}^n) \right. \\
&\quad \left. - \left(\sum_{k=1}^{N_d} v_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(v_j^n) \ln(v_{i,k}^n) - \sum_{k=1}^{N_d} v_{i,k-\frac{1}{2}} D_{k-\frac{1}{2}}(v_j^n) \ln(v_{i,k}^n) \right) \right] \\
&= -\Delta t \frac{1}{(e^n)^2} \sum_{i<j} a_{ij} \sum_{k=1}^{N_d-1} h v_{i,k+\frac{1}{2}} v_{j,k+\frac{1}{2}} \left| D_{k+\frac{1}{2}}(\ln(v_i^n)) - D_{k+\frac{1}{2}}(\ln(v_j^n)) \right|^2 \\
&\quad + \Delta t \frac{(e')^n}{e^n} \sum_{i=1}^N \ln(v_{i,N_d}^n) \left(\frac{\phi_i^n}{(e')^n} - v_{i,N_d+\frac{1}{2}} \right),
\end{aligned}$$

and for the drift term :

$$T_{drift,ent} = \Delta t \frac{(e')^n}{e^n} \left[\sum_{i=1}^N v_{i,N_d+\frac{1}{2}} \ln(v_{i,N_d}^n) - E^n - \sum_{i=1}^N \sum_{k=1}^{N_d-1} \Delta x x_{k+\frac{1}{2}} \tilde{v}_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(\ln(v_i^n)) \right].$$

We can see that the first part of the drift term compensate a part of the diffusion term. So, to sum up, by summing all terms we get, by "cleaning" the a_{ij} -term in a similar fashion as for the a^* -term :

$$\begin{aligned}
& \left(1 - \frac{\Delta t(e')^n}{e^{n-1} + \Delta t(e')^n}\right) \left[E^n - E^{n-1} \right] + \min_{i,j} a_{ij} \sum_{i=1}^N \sum_{k=1}^{N_d-1} \Delta x v_{i,k+\frac{1}{2}} \left| D_{k+\frac{1}{2}}(\ln(v_i^n)) \right|^2 \\
& \leq \Delta t \frac{(e')^n}{e^n} \left[\sum_{i=1}^N \frac{\phi_i^n}{(e')^n} \ln(v_{i,N_d}) - E^n - \sum_{i=1}^N \sum_{k=1}^{N_d-1} \Delta x x_{k+\frac{1}{2}} \tilde{v}_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(\ln(v_i^n)) \right]. \quad (13)
\end{aligned}$$

However, if $\min(v_{i,k}^n, v_{i,k+1}^n) > 0$, we have:

$$\tilde{v}_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(\ln(v_i^n)) = \frac{v_{i,k+\frac{1}{2}}^n}{\sum_j v_{j,k+\frac{1}{2}}^n} D_{k+\frac{1}{2}}(v_i^n).$$

Summing over all species yields zero for the previous term, therefore :

$$\begin{aligned}
& \left(1 - \frac{\Delta t(e')^n}{e^{n-1} + \Delta t(e')^n}\right) \left[E^n - E^{n-1} \right] + \min_{i,j} a_{ij} \sum_{i=1}^N \sum_{k=1}^{N_d-1} \Delta x v_{i,k+\frac{1}{2}} \left| D_{k+\frac{1}{2}}(\ln(v_i^n)) \right|^2 \\
& \leq \Delta t \frac{(e')^n}{e^n} \left[\sum_{i=1}^N \frac{\phi_i^n}{(e')^n} \ln(v_{i,N_d}) - E^n \right]. \quad (14)
\end{aligned}$$

4 Compactness and convergence

4.1 Reconstruction operators

Let us denote $I_k := (x_{k-\frac{1}{2}}, x_{k+\frac{1}{2}})$ and $\Theta_{k+\frac{1}{2}} := (x_{k-1}, x_{k+1})$ (unless $k = 1, N_d$ for the latter, in which case we take the boundaries of $(0, 1)$ being the cell centered in x_k and the "diamond cells", being intervals centered in $x_{k+\frac{1}{2}}$. Both of these sequences of the closure of these intervals are a partition of $(0, 1)$:

$$\tau := (\overline{I}_k)_{k \in [|1, N_d|]} \quad \text{and} \quad \epsilon := (\overline{\Theta}_{k+\frac{1}{2}})_{k \in [|0, N_d|]}.$$

We define the piecewise constant interpolation function:

$$\begin{aligned}
\Pi_{\tau, \Delta t}(\mathbf{c})(t, x) &:= \sum_{k=1}^{N_d} \sum_{n=1}^{N_T} c_k^n \mathbf{1}_{x \in I_k} \mathbf{1}_{t \in (t_{n-1}, t_n]}, \\
\Pi_{\epsilon, \Delta t}^{log}(\mathbf{c})(t, x) &:= \sum_{k=0}^{N_d} \sum_{n=1}^{N_T} c_{k+\frac{1}{2}}^n \mathbf{1}_{x \in E_{k+\frac{1}{2}}} \mathbf{1}_{t \in (t_{n-1}, t_n]}, \\
\Pi_{\epsilon, \Delta t}^{norm}(\mathbf{c})(t, x) &:= \sum_{k=0}^{N_d} \sum_{n=1}^{N_T} \tilde{c}_{k+\frac{1}{2}}^n \mathbf{1}_{x \in E_{k+\frac{1}{2}}} \mathbf{1}_{t \in (t_{n-1}, t_n]},
\end{aligned}$$

with $c_{k+\frac{1}{2}}$ being the log-mean in the sense of Equation 2 and $\tilde{c}_{k+\frac{1}{2}}$ being the arithmetic-mean in the sense of Equation 3, and the derivative reconstruction operator :

$$\nabla_{\tau, \Delta t}(\mathbf{c})(t, x) := \sum_{k=0}^{N_d} \sum_{n=1}^{N_T} D_{k+\frac{1}{2}}(c^n) \mathbf{1}_{x \in E_k} \mathbf{1}_{t \in (t_{n-1}, t_n]}.$$

The discrete $L^2((0, 1))$ scalar product for the derivatives becomes :

$$\int_0^1 \nabla_\tau(\mathbf{f}) \nabla_\tau(\mathbf{g}) = \sum_{k=0}^{N_d} \Delta x D_{k+\frac{1}{2}}(f) D_{k+\frac{1}{2}}(g).$$

4.2 $L^2(0, T; L^2(0, 1))^N$ estimate

By the stability of \mathcal{A} , we immediately have :

$$\sum_{i=1}^N \iint_{Q_T} |\Pi_{\tau, \Delta t}(v_i)|^2 \leq T.$$

4.3 $L^2(0, T; H^1(0, 1))^N$ estimate

This one is trickier but thanks to the entropy structure, we manage to pull through.
Mainly,

$$\begin{aligned} \sum_{i=1}^N \iint_{Q_T} \left| \nabla_{\tau, \Delta t}(\sqrt{v_i}) \right|^2 &= \sum_{i=1}^N \sum_{n=1}^{N_T} \sum_{k=0}^{N_d} \Delta t \Delta x D_{k+\frac{1}{2}} \left(\sqrt{v_{i,k}^n} \right)^2 \\ &= \frac{1}{4} \sum_{i=1}^N \sum_{n=1}^{N_T} \sum_{k=0}^{N_d-1} \Delta t \Delta x \bar{v}_{i,k+\frac{1}{2}}^n D_{k+\frac{1}{2}} (\ln(v_{i,k}^n))^2 + \sum_{i=1}^N \sum_{n=1}^{N_T} \Delta t \frac{\Delta x}{2} D_{N_d+\frac{1}{2}} \left(\sqrt{v_{i,N_d}^n} \right)^2, \end{aligned}$$

with :

$$\bar{v}_{i,k+\frac{1}{2}}^n = 4 \left(\frac{D_{k+\frac{1}{2}}(\sqrt{v_i^n})}{D_{k+\frac{1}{2}}(\ln(v_i^n))} \right)^2.$$

Given that for any $a < b$, by Cauchy-Schwarz's inequality :

$$4(\sqrt{b} - \sqrt{a})^2 = \left(\int_a^b \frac{dx}{\sqrt{x}} \right)^2 \leq \left(\int_a^b dx \right) \left(\int_a^b \frac{dx}{x} \right) = (b-a)(\ln(b) - \ln(a)),$$

we have :

$$\bar{v}_{i,k+\frac{1}{2}}^n \leq v_{i,k+\frac{1}{2}}^n.$$

Using the entropy inequality, we have :

$$\begin{aligned} \sum_{i=1}^N \iint_{Q_T} |\nabla_{\tau, \Delta t}(\sqrt{v_i})|^2 &\leq \frac{1}{4 \min a_{ij}} \sum_{n=1}^{N_T} \left(\left(1 - \frac{\Delta t (e')^n}{e^{n-1} + \Delta t (e')^n} \right) [E^{n-1} - E^n] \right. \\ &\quad \left. + \Delta t \frac{(e')^n}{e^n} \left[\sum_{i=1}^N \frac{\phi_i^n}{(e')} \ln(v_{i,N_d}^n) - E^n \right] \right) + \frac{1}{4 \min a_{ij}} \sum_{i=1}^N \sum_{n=1}^{N_T} \Delta t \frac{\Delta x}{2} D_{N_d+\frac{1}{2}} \left(\sqrt{v_{i,N_d}^n} \right)^2 \\ &\leq \frac{NT}{4 \min a_{ij}} \left(\frac{1}{e} + \frac{\Delta x}{2} \right). \end{aligned}$$

We conclude by noting that for any $k \in [|0, N_d|]$ and any positive real couple (a, b) :

$$\begin{aligned} 2(\sqrt{b} - \sqrt{a}) &= \frac{2}{\sqrt{a} + \sqrt{b}}(b - a) \\ &\geq (b - a) \text{ if } a, b \leq 1. \end{aligned}$$

4.4 $H^1(0, T; (H^1(0, 1))')^N$ estimate

Defining the discrete dual norm :

$$\|v\|_{-1} = \left\{ \sup_{\psi} \int_0^1 \Pi_\tau v \Pi_\tau \psi , \quad \|\Pi_\tau \psi\|_{L^2(0,1)}^2 + \|\nabla_\tau \psi\|_{L^2(0,1)}^2 = 1 \right\}.$$

Let us therefore take a vector $\psi \in \mathbb{R}^{N_d}$ such that $\|\Pi_\tau \psi\|_{L^2(0,1)}^2 + \|\nabla_\tau \psi\|_{L^2(0,1)}^2 = 1$. Multiplying it by $\Delta t \Pi_\tau \psi$ for a given n then integrating over $(0, 1)$ yields :

$$\int_0^1 \Pi_\tau (v_i^n - v_i^{n-1}) \Pi_\tau \psi = T_{diff, a^*}^\psi + T_{diff, a_{ij} - a^*}^\psi + T_{drift}^\psi.$$

Let us start by looking at the a^* terms. We have first :

$$\begin{aligned} T_{diff, a^*}^\psi &:= \frac{\Delta t a^*}{(e^n)^2} \left[\sum_{k=1}^{N_d} \psi_k D_{k+\frac{1}{2}}(v_i^n) - \sum_{k=1}^{N_d} \psi_k D_{k-\frac{1}{2}}(v_i^n) \right] \\ &= \frac{\Delta t a^*}{(e^n)^2} \left[-h D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\psi) + D_{N_d+\frac{1}{2}}(v_i^n) \psi_{N_d} \right], \end{aligned}$$

and secondly :

$$\begin{aligned} T_{diff, a_{ij} - a^*}^{\psi, a^* term} &:= \frac{\Delta t a^*}{(e^n)^2} \sum_{j=1}^N \left[- \left(\sum_{k=1}^{N_d} v_{j,k+\frac{1}{2}}^n D_{k+\frac{1}{2}}(v_i^n) \psi_k - \sum_{k=1}^{N_d} v_{j,k-\frac{1}{2}}^n D_{k-\frac{1}{2}}(v_i^n) \psi_k \right) \right. \\ &\quad \left. + \left(\sum_{k=1}^{N_d} v_{i,k+\frac{1}{2}}^n D_{k+\frac{1}{2}}(v_j^n) \psi_k - \sum_{k=1}^{N_d} v_{i,k-\frac{1}{2}}^n D_{k-\frac{1}{2}}(v_j^n) \psi_k \right) \right] \\ &= \frac{\Delta t a^*}{(e^n)^2} \left[h \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\psi) \sum_j (v_{j,k+\frac{1}{2}}) - h \sum_{k=1}^{N_d-1} v_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(\psi) \sum_j (D_{k+\frac{1}{2}}(v_j^n)) \right. \\ &\quad \left. + \psi_{N_d} D_{N_d+\frac{1}{2}}(v_i^n) \sum_j (v_{j,N_d+\frac{1}{2}}) - \psi_{N_d} v_{i,N_d+\frac{1}{2}}^n \sum_j (D_{N_d+\frac{1}{2}}(v_j^n)) \right] \\ &= \frac{\Delta t a^*}{(e^n)^2} h \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\psi) \sum_j (v_{j,k+\frac{1}{2}}). \end{aligned}$$

Therefore the a^* contribution yields by Cauchy-Schwarz's inequality :

$$\begin{aligned}
T_{diff,a^*}^\psi &= \frac{\Delta t a^*}{(e^n)^2} h \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\psi) \left[\sum_j (v_{j,k+\frac{1}{2}}) - 1 \right] \\
&\leq \frac{\Delta t a^*}{(e^n)^2} \left[\sum_{k=1}^{N_d-1} h D_{k+\frac{1}{2}}(v_i^n)^2 \left(\sum_j (v_{j,k+\frac{1}{2}}) - 1 \right)^2 \right]^{\frac{1}{2}} \left[\sum_{k=1}^{N_d-1} h D_{k+\frac{1}{2}}(\psi)^2 \right]^{\frac{1}{2}} \\
&\leq \frac{\Delta t a^*}{(e^n)^2} \|\nabla_\tau v_i^n\|_{L^2(0,1)} \|\nabla_\tau \psi\|_{L^2(0,1)}.
\end{aligned}$$

For the a_{ij} term, similarly :

$$\begin{aligned}
T_{diff,a_{ij}-a^*}^{\psi,a_{ij}term} &:= \frac{\Delta t}{(e^n)^2} \left[h \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\psi) \sum_j (a_{ij} v_{j,k+\frac{1}{2}}) - h \sum_{k=1}^{N_d-1} v_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(\psi) \sum_j (a_{ij} D_{k+\frac{1}{2}}(v_j^n)) \right] \\
&\quad + \Delta t \psi_{N_d} \frac{(e')^n}{e^n} \left[\frac{\phi_i^n}{(e')^n} - v_{i,N_d+\frac{1}{2}} \right].
\end{aligned}$$

The remaining drift term yields :

$$T_{drift}^\psi := \Delta t \frac{(e')^n}{e^n} \left[-h \sum_{k=1}^{N_d-1} x_{k+\frac{1}{2}} \tilde{v}_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(\psi) + \psi_{N_d} v_{i,N_d+\frac{1}{2}} - \sum_{k=1}^{N_d} \psi_k \Delta x v_{i,k}^{n-1} \right].$$

Summing both terms and heavily using Cauchy Schwarz's inequality :

$$\begin{aligned}
T_{remaining} &\leq \frac{\Delta t}{(e^n)^2} \left[(e^n)^2 \sum_{j=1}^N a_{ij} (v_{j,k+\frac{1}{2}}^n \|\nabla_\tau v_i^n\|_{L^2(0,1)} - v_{i,k+\frac{1}{2}}^n \|\nabla_\tau v_j^n\|_{L^2(0,1)}) \right] \|\nabla_\tau \psi\|_{L^2(0,1)} \\
&\quad + \frac{\Delta t (e')^n}{e^n} \left[\|\Pi_\epsilon^{ari}(xv_i^n(x))\|_{L^2(0,1)} \|\nabla_\tau(\psi)\|_{L^2(0,1)} + \left(\|\Pi_\tau(v_i^{n-1})\|_{L^2(0,1)} + \frac{\phi_i}{(e')^n} \right) \|\Pi_\tau(\psi)\|_{L^2(0,1)} \right].
\end{aligned}$$

In conclusion, we have :

$$\left\| \frac{\Pi_\tau(v_i^n - v_i^{n-1})}{\Delta t} \right\|_{-1} \leq C_{N,T,a_{ij}}.$$

5 Convergence toward the weak solution

We can apply a discrete Aubin-Lions theorem to obtain for a sequences of discretizations both in time and space, where both Δt and Δx goes to 0. Indeed, noting that each v_i^n is in L^∞ , we have :

$$\begin{aligned}
\Pi_{\tau_m, \Delta t_m}(v_i) &\xrightarrow[m \rightarrow 0]{} v_i \quad \text{in } L^p[0, T; L^p(0, 1)] \text{ for } p \in [1, +\infty), \\
\nabla_{\tau_m, \Delta t_m}(v_i) &\xrightarrow[m \rightarrow 0]{} \partial_x v_i \quad \text{in } L^2[0, T; L^2(0, 1)].
\end{aligned}$$

In addition, to prove convergence toward the weak solution, we need the convergence on the edges. Noting that:

$$\begin{aligned}
\|\Pi_{\tau,\Delta t}(v_i) - \Pi_{\epsilon,\Delta t}^{\log}(v_i)\|_{L^1(0,1)} &= \sum_{n=1}^{N_T} \Delta t \sum_{k=1}^{N_d} h_{k-\frac{1}{2}} |v_{i,k}^n - v_{i,k-\frac{1}{2}}^n| + \Delta x |v_{i,k+\frac{1}{2}}^n - v_{i,k}^n| \\
&\leq \sum_{n=1}^{N_T} \Delta t \sum_{k=1}^{N_d} h_{k-\frac{1}{2}}^2 D_{k-\frac{1}{2}}(v_i^n) + \Delta x^2 D_{k+\frac{1}{2}}(v_i^n) \\
&\leq 2(\max_k \Delta x) \sqrt{T} \|\nabla_{\tau,\Delta t}(v_i)\|_{L^2(0,1)},
\end{aligned}$$

which goes to zero as the discretization refines. Therefore, as $\Pi_{\tau,\Delta t}(v_i) \rightarrow v_i$ in any $L^p((0,1) \times (0,T))$. By Holdér inequality, this implies that $\Pi_{\epsilon,\Delta t}^{\log}(v_i) \rightarrow v_i$ in any $L^p((0,1) \times (0,T))$.

In particular, from the partial converse Lebesgue theorem, the convergence occurs almost everywhere, and so as the discretization refines:

$$\sum_{j=1}^N v_{j,k \pm \frac{1}{2}} \rightarrow 1.$$

Which in turns yields :

$$\Pi_{\epsilon,\Delta t}^{\text{norm}}(v_i) \rightarrow v_i \text{ a.e.}$$

As the previous function is uniformly bounded, the convergence also occurs in any $L^p((0,1) \times (0,T))$.

These results allow the discrete WF to converge to the continuous one.

Indeed, let us take $\psi \in \mathcal{C}_c^1([0,T] \times [0,1])$ and $\Psi \in \mathbb{R}^{N_T \times N_d}$ be the vector of its interpolated values on the discrete spatial and temporal mesh.

For the time-dependent term, multipliyng by $\Delta t \Psi_k^{n-1}$ then summing over (n, k) yields :

$$\begin{aligned}
T_{\text{time}}^\psi &:= \sum_{k=1}^{N_d} \Delta x \left[\sum_{n=1}^{N_T} v_{i,k}^n \Psi_k^{n-1} - \sum_{n=1}^{N_T} v_{i,k}^{n-1} \Psi_k^{n-1} \right] \\
&= \sum_{k=1}^{N_d} \left[-v_{i,k}^0 \Psi_k^0 + \sum_{n=1}^{N_T-1} v_{i,k}^n (\Psi_k^{n-1} - \Psi_k^n) + v_{i,k}^{N_T} \Psi_k^{N_T-1} \right] \\
&= - \int_0^1 \Pi_\tau(v_i^0) \Pi_\tau(\Psi^0) + \iint_{Q_T} \Pi_{\tau,\Delta t}(v_i)(\nabla_{\Delta t} \Pi_\tau)(\Psi) + \int_0^1 \Pi_\tau(v_i^{N_T}) \Pi_\tau(\Psi^{N_T-1}),
\end{aligned}$$

where we defined the hybrid operator $(\nabla_{\Delta t} \Pi_\tau)$ as :

$$\begin{aligned}
\forall f \in L^\infty(Q_T) \quad (\nabla_{\Delta t} \Pi_\tau)(f) &:= \sum_{n=1}^{N_T-1} \frac{\Pi_\tau(f^n) - \Pi_\tau(f^{n-1})}{\Delta t_n} \mathbf{1}_{t \in (t_{n-1}, t_n]} \\
&= \sum_{n=1}^{N_T-1} \sum_{k=1}^{N_d} \frac{f_k^n - f_k^{n-1}}{\Delta t} \mathbf{1}_{x \in I_k} \mathbf{1}_{t \in (t_{n-1}, t_n]}.
\end{aligned}$$

As we have uniformly :

$$\begin{aligned}\Pi_\tau(\Psi^0) &\xrightarrow[h \rightarrow 0]{} \psi(0, .), \\ \Pi_\tau(\Psi^{N_T-1}) &\xrightarrow[(h, \Delta t) \rightarrow (0, 0)]{} \psi(1, .), \\ (\nabla_{\Delta t} \Pi_\tau)(\Psi) &\xrightarrow[(h, \Delta t) \rightarrow (0, 0)]{} \partial_t \psi,\end{aligned}$$

and

$$\Pi_{\tau, \Delta t}(v_i) \xrightarrow[(h, \Delta t) \rightarrow (0, 0)]{} v_i,$$

the continuous and discrete weak formulation coïncide for the T_{time} -term.

For the first a^* term :

$$\begin{aligned}T_{diff, a^*}^\psi &= \sum_{n=1}^{N_T} \frac{a^* \Delta t}{(e^n)^2} \left[\sum_{k=1}^{N_d} D_{k+\frac{1}{2}}(v_i^n) \Psi_k^{n-1} - \sum_{k=1}^{N_d} D_{k-\frac{1}{2}}(v_i^n) \Psi_k^{n-1} \right] \\ &= \sum_{n=1}^{N_T} \frac{a^* \Delta t}{(e^n)^2} \left[-\Delta x \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\Psi^{n-1}) + D_{N_d+\frac{1}{2}}(v_i^n) \Psi_{N_d}^{n-1} \right] \\ &= - \iint_{Q_T} \frac{a^*}{\Pi_{\Delta t}(e^2)} \nabla_{\tau, \Delta t}(v_i) \nabla_{\tau, \Delta t}(\Psi) + \int_0^1 \frac{a^*}{\Pi_{\Delta t}(e^2)} \nabla_{\tau, \Delta t}(v_i) \Pi_\tau(\Psi_{N_d}).\end{aligned}$$

The other a^* term yields :

$$\begin{aligned}T_{diff, a_{ij} - a^*}^{a^*, \psi} &= -a^* \sum_{n=1}^{N_T} \frac{\Delta t}{(e^n)^2} \left[\sum_{k=1}^{N_d} \left(\left(\sum_j v_{j, k+\frac{1}{2}} \right) D_{k+\frac{1}{2}}(v_i^n) - v_{i, k+\frac{1}{2}} \sum_j (D_{k+\frac{1}{2}}(v_j^n)) \right) \Psi_k^{n-1} \right. \\ &\quad \left. - \sum_{k=1}^{N_d} \left(\left(\sum_j v_{j, k-\frac{1}{2}} \right) D_{k-\frac{1}{2}}(v_i^n) - v_{i, k-\frac{1}{2}} \sum_j (D_{k-\frac{1}{2}}(v_j^n)) \right) \Psi_k^{n-1} \right] \\ &= -a^* \sum_{n=1}^{N_T} \frac{\Delta t}{(e^n)^2} \left[-\Delta x \sum_{k=1}^{N_d-1} D_{k+\frac{1}{2}}(v_i^n) D_{k+\frac{1}{2}}(\Psi_{n-1}) + D_{N_d+\frac{1}{2}}(v_i^n) \Psi_{N_d}^{n-1} \right].\end{aligned}$$

We can therefore see that the a^* terms cancels each other out.

For the remaining a_{ij} term :

$$\begin{aligned}T_{diff, a_{ij} - a^*}^{a^*, \psi} &= \sum_{n=1}^{N_T} \frac{\Delta t}{(e^n)^2} \left[-h \sum_{k=1}^{N_d-1} \sum_{j=1}^N a_{ij} (v_{j, k+\frac{1}{2}}^n D_{k+\frac{1}{2}}(v_i^n) - v_{i, k+\frac{1}{2}}^n D_{k+\frac{1}{2}}(v_j^n)) D_{k+\frac{1}{2}}(\Psi^{n-1}) \right. \\ &\quad \left. + (e')^n e^n \left(\frac{\phi_i^n}{(e')^n} - v_{i, N_d+\frac{1}{2}} \right) \Psi_{N_d}^{n-1} \right] \\ &= - \iint_{Q_T} \frac{1}{\Pi_{\Delta t}(e^2)} \sum_{j=1}^N a_{ij} \left(\Pi_{\epsilon, \Delta t}^{log}(v_j) \nabla_{\tau, \Delta t}(v_i) - \Pi_{\epsilon, \Delta t}^{log}(v_i) \nabla_{\tau, \Delta t}(v_j) \right) \\ &\quad + \int_0^T \frac{\Pi_{\Delta t}(e')}{\Pi_{\Delta t}(e)} \left(\frac{\Pi_{\Delta t}(\phi_i)}{\Pi_{\Delta t}(e)} - \Pi_{\Delta t}(v_i^{N_d+\frac{1}{2}}) \right) \Pi_{\Delta t}(\Psi_{N_d}).\end{aligned}$$

The drift terms yields with similar calculation:

$$\begin{aligned}
T_{drift}^\psi &:= \sum_{n=1}^{N_T} \frac{\Delta t(e')^n}{e^n} \left[-h \sum_{k=1}^{N_d-1} x_{k+\frac{1}{2}} \tilde{v}_{i,k+\frac{1}{2}} D_{k+\frac{1}{2}}(\Psi^{n-1}) + v_{i,N_d+\frac{1}{2}} \Psi_{N_d}^{n-1} - \sum_{k=1}^{N_d} \Delta x v_{i,k}^{n-1} \Psi_k^{n-1} \right] \\
&= - \iint_{Q_T} \frac{\Pi_{\Delta t}(e')}{\Pi_{\Delta t}(e)} \Pi_{\epsilon, \Delta t}^{norm}(xv_i) \nabla_{\tau, \Delta t}(\Psi) + \Pi_{\tau, \Delta t}(v_i) \Pi_{\tau, \Delta t}(\Psi) \\
&\quad + \int_0^T \frac{\Pi_{\Delta t}(e')}{\Pi_{\Delta t}(e)} \Pi_{\Delta t}(v_i^{N_d+\frac{1}{2}}) \Pi_{\Delta t}(\Psi_{N_d}).
\end{aligned}$$

While the second term gets cancelled out by half of the previous term, the first term converges, when both $(\Delta t, \Delta x)$ goes to 0, to :

$$- \iint_{Q_T} \frac{e'}{e} (x \partial_x \psi + \psi) v_i.$$

Finally, the whole thing converges to (1)

6 Case of constant flux

In case the flux $\phi_i(t)$ are all constant, set to be $\bar{\phi}_i$, defining for each specie

$$f_i = \frac{\bar{\phi}_i}{V}, \quad \text{with } \forall t \in (0, T) \quad V := e'(t) \quad \text{and therefore } e(t) = e_0 + Vt.$$

6.1 Entropy decay

We then have, by defining the entropy $\overline{E^n}$ as :

$$\begin{aligned}
\overline{E^n} &= E^n - \sum_i f_i \ln(f_i) - \sum_{i,k} \Delta x (\ln(f_i) + 1) (v_{i,k}^n - f_i) \\
&= \sum_{i,k} v_{i,k}^n \ln\left(\frac{v_{i,k}^n}{f_i}\right).
\end{aligned}$$

We then follow the same approach as in Section (3.7) to deduce a new entropy inequality.

Setting $h(v) := v \ln(v)$ the kernel function for the discrete entropy E , noting that $\bar{h}(v) = h(v) - h(f_i) - h'(f_i)(v - f_i)$, we make the following observations :

- Both h and \bar{h} are convex with $\bar{h}' = h' - h'(f_i)$,
- $\forall v \in \mathcal{A} \quad \sum_i \bar{h}(v_i) \leq \sum_i h'(f_i) = 0$,
- The definition of each $v_{i,k \pm \frac{1}{2}}$ does not change in the sense that: $v_{i,k \pm \frac{1}{2}} D_{k \pm \frac{1}{2}}(\bar{h}(v)) = D_{k \pm \frac{1}{2}}(v)$,

- $D_{k \pm \frac{1}{2}}(\bar{h}(v)) = D_{k \pm \frac{1}{2}}(h(v)).$

These observations allow us to reproduce the computations done in (3.7) to arrive at :

$$\begin{aligned} & \left(1 - \frac{\Delta t V}{e_0 + n \Delta t V}\right) \left[\bar{E}^n - \bar{E}^{n-1} \right] + \min_{i,j} a_{ij} \sum_{i=1}^N \sum_{k=1}^{N_d-1} \Delta x v_{i,k+\frac{1}{2}} \left| D_{k+\frac{1}{2}}(h'(v_i^n)) \right|^2 \\ & \leq \frac{\Delta t V}{e_0 + n \Delta t V} \left[\sum_{i=1}^N f_i \bar{h}'(v_{i,N_d}^n) - \bar{E}^n \right]. \end{aligned}$$

The convexity of \bar{h} yields :

$$\sum_i f_i \bar{h}'(v_{i,N_d}^n) \leq \sum_i \bar{h}(f_i) = 0.$$

Therefore, we arrive at:

$$\bar{E}^n \leq \left(1 - \frac{\Delta t V}{e_0 + n \Delta t V}\right) \bar{E}^{n-1},$$

and finally :

$$\bar{E}^n \leq \frac{e_0}{e_0 + n \Delta t V} \bar{E}^0. \quad (15)$$

This shows that the modified entropy decreases at a rate of at most $\frac{1}{n \Delta t}$

6.2 Long term behaviour

From the mass conservation equation (10), given constant fluxes and writing for simplicity constant discretization steps both in time $\Delta t = \Delta t$ and in space $\Delta x =: \Delta x$, we get by summation over all time steps:

$$\sum_{k=1}^{N_d} \Delta x \left(e_0 + N_T \Delta t V \right) v_{i,k}^{N_T} = e_0 \sum_{k=1}^{N_d} v_{i,k}^0 + N_T \Delta t (V f_i).$$

By denoting $\bar{v}_i := \sum_{k=1}^{N_d} \Delta x v_{i,k}$ as the mass related to the specie i , and recalling that $T = N_T \Delta t$, we have therefore :

$$|\bar{v}_i^{N_T} - f_i| \leq \frac{e_0}{e_0 + TV} |v_i^0 - f_i|.$$

This shows the convergence of the total mass to the flux profile at a rate $\frac{1}{T}$. But in fact, we can show that the concentrations $v_{i,k}$ all converges toward the flux at a slower rate, all over the spatial domain.

Let us use the following Csizar-Kullback inequality applied to our particular settings :

Lemma 6.1. Let $g \in L^1(0, 1)$ be a positive function such that $\|g\|_{L^1(0,1)} = 1$. Then :

$$\|g - 1\|_{L^1(0,1)}^2 \leq 2 \int_0^1 g(x) \ln(g(x)) dx.$$

Proof. Let us define the functional h such that :

$$h(g) := g \ln(g) - g + 1.$$

We have by Taylor's expansion :

$$\begin{aligned} h(g) &= h(1) + h'(1)(g - 1) + \int_1^g h''(u)(g - u) du \\ &= h(1) + h'(1)(g - 1) + (g - 1)^2 \int_0^1 h''(1 + s(g - 1))(1 - s) ds \quad \text{changing variables } u = 1 + s(g - 1) \\ &= (g - 1)^2 \int_0^1 \frac{1 - s}{1 + s(g - 1)} ds. \end{aligned}$$

By Fubini :

$$\begin{aligned} H(g) &:= \int_0^1 h(g(x)) dx \\ &= \int_0^1 (1 - s) \left(\int_0^1 \frac{(g(x) - 1)^2}{1 + s(g(x) - 1)} dx \right) ds, \end{aligned}$$

we almost recognize the square of an L^1 -norm. According to Cauchy Schwarz's inequality, for any $s \in (0, 1)$:

$$\begin{aligned} \left(\int_0^1 |g(x) - 1| dx \right)^2 &\leq \left(\int_0^1 \frac{(g(x) - 1)^2}{1 + s(g(x) - 1)} dx \right) \left(\int_0^1 (1 + s(g(x) - 1)) dx \right) \\ &= \int_0^1 \frac{(g(x) - 1)^2}{1 + s(g(x) - 1)}, \quad \text{due to } \|g\|_{L^1(0,1)} = 1. \end{aligned}$$

Therefore we arrive at the desired result:

$$H(g) \geq \frac{1}{2} \|g - 1\|_{L^1(0,1)}^2.$$

□

Applying this lemma to the piecewise constant interpolation function as define in Section 4:

$$\frac{\Pi_\tau(v_i^n)}{\bar{v}_i^n} = \frac{\Pi_\tau(v_i^n)}{\int_0^1 \Pi_\tau(v_i^n)(x) dx},$$

we have, recalling that $\bar{v}_i^n \leq 1$,

$$\begin{aligned}
\|v_{i,.}^n - \bar{v}_i^n\|_{L^1(0,1)}^2 &\leq \|v_{i,.}^n - \bar{v}_i^n\|_{L^1(0,1)}^2 \frac{\bar{v}_i^n}{(\bar{v}_i^n)^2} \\
&\leq 2 \sum_{k=1}^{N_d} \Delta x v_{i,k}^n \ln\left(\frac{v_{i,k}^n}{\bar{v}_i^n}\right) \\
&= 2 \sum_{k=1}^{N_d} \Delta x v_{i,k}^n \ln\left(\frac{v_{i,k}^n}{f_i}\right) + 2 \left(\sum_{k=1}^{N_d} \Delta x v_{i,k}^n \right) \ln\left(\frac{f_i}{\bar{v}_i^n}\right).
\end{aligned} \tag{16}$$

Summing over i :

$$\sum_{i=1}^N \|v_{i,.}^n - \bar{v}_i^n\|_{L^1(0,1)}^2 \leq 2\bar{E}^n + 2 \sum_{i=1}^N \bar{v}_i^n \ln\left(\frac{f_i}{\bar{v}_i^n}\right).$$

On one hand, the modified entropy is decreasing at least by a factor of $\frac{1}{T}$. On the other hand, by the conservation of mass, we can deduce a uniform lower bound for any \bar{v}_i^n . Indeed, we have from the mass conservation law, setting $\alpha_n := \frac{e_0}{e_0 + nV\Delta t}$

$$\bar{v}_i^n = \alpha_n \bar{v}_i^0 + (1 - \alpha_n) f_i.$$

This implies that \bar{v}_i^n goes either increasingly or decreasingly (depending on $\bar{v}_i^0 \geq f_i$ or $\bar{v}_i^0 \leq f_i$) towards f_i . This means :

$$\forall n \in \mathbb{N} \quad \min(\bar{v}_i^0, f_i) \leq \bar{v}_i^n \leq \max(\bar{v}_i^0, f_i).$$

Setting $C = \min_i(\bar{v}_i^0, f_i)$ over all species, we have

$$|\ln(f_i) - \ln(\bar{v}_i^n)| \leq \frac{1}{C} |\bar{v}_i^n - f_i|,$$

and therefore :

$$\begin{aligned}
\sum_{i=1}^N \|v_{i,.} - f_i\|_{L^1(0,1)}^2 &\leq \sum_{i=1}^N \|v_{i,.} - \bar{v}_i^n\|_{L^1(0,1)}^2 + \sum_{i=1}^N \sum_{j=1}^N |\bar{v}_j^n - f_j|^2 \\
&\leq 2 \frac{e_0}{e_0 + n\Delta t V} \bar{E}^0 + 2 \frac{e_0}{e_0 + n\Delta t V} \frac{|v_i^0 - f_i|}{C} + N \left(\frac{e_0}{e_0 + n\Delta t V} \sum_{j=1}^N |v_j^0 - f_j| \right)^2.
\end{aligned}$$

This implies a L^1 -error decreasing at most as $T^{-\frac{1}{2}}$.

7 Numerical Simulation : Piecewise Constant Flux

We implemented our simulation on the programming language *Julia*, using the packages *LinearAlgebra*, *NLsolve*, *ForwardDiff*, *Plots* and *LaTeXStrings*. The code is available at https://github.com/NicoShol/1D_entropyScheme_xdiff.

7.1 Initial Profile

We chose $N = 4$ species for this numerical simulation, with an initial concentration profile illustrated in Figure (7.1). For the fluxes $(\Phi_i)_i$, we chose to use piecewise constant flux as shown in Figure (7.1). The discretization parameters are displayed in Table (1)

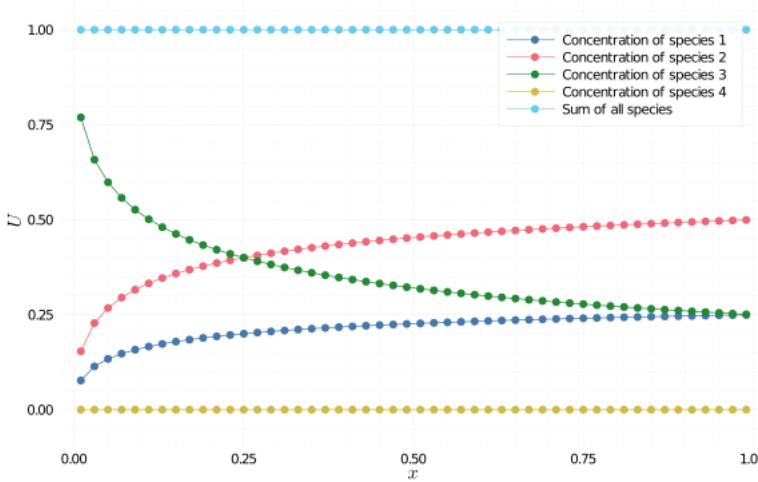


Figure 3: Initial Profile

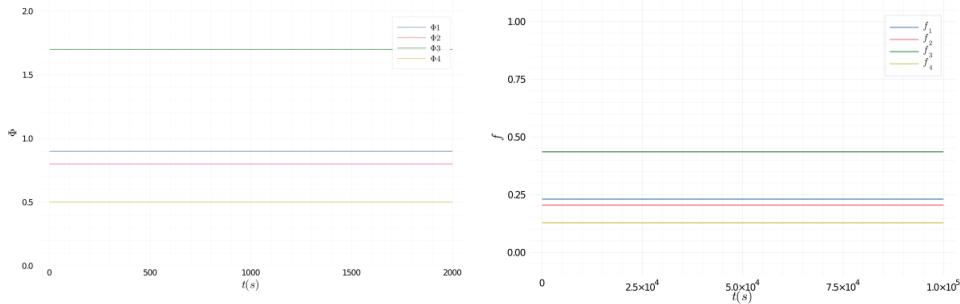


Figure 4: Flux

N	4
N_T	200
Δt	1
N_d	50
Δx	0.02

Table 1: Discretization Parameters

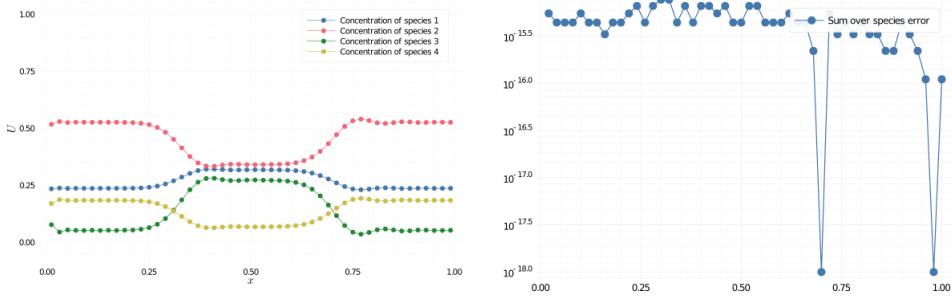


Figure 5: Final Profile

Figure (7.1) shows the profile at $T = 200s$, and the sum of all species along the spatial dimension.

We first note the stability of the summation to 1 up to machine precision 10^{-15} (we also rounded up all values below 10^{-18}). This is to be expected for any discretization $(\Delta x, \Delta t) \in \mathbb{R}_+ \times \mathbb{R}_+$.

The piecewise constant flux (split into thirds) is also replicated in the final profile, confirming our intuition.

7.2 Mass conservation

We aim here to verify the mass conservation equation (10) recalled below:

$$\sum_{k=1}^{N_d} e^n \Delta x v_{i,k}^n - \sum_{k=1}^{N_d} e^{n-1} \Delta x v_{i,k}^{n-1} = \phi_i^n \Delta t.$$

Figure (7.2) illustrate the evolution of the mass along the scheme. We can see that the conservation of mass is true and fluctuate up to a tolerance of 10^{-9} , for all 4 masses (only the specie 4 is illustrated here for clarity, as all species have similar behaviour). The error does not seem to accumulate as the times increases.

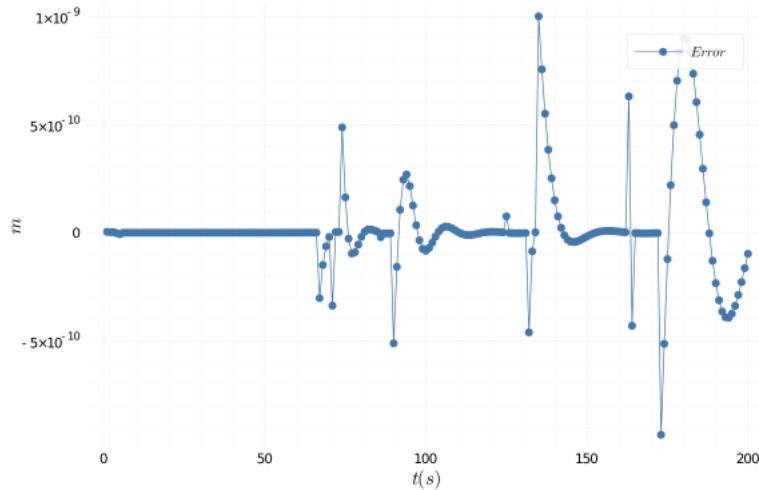


Figure 6: Mass for species 4 (other yields similar profiles)

7.3 Entropy

This section illustrate a slightly less restricted version of Equation (14):

$$\left(1 - \frac{\Delta t(e')^n}{e^{n-1} + \Delta t(e')^n}\right) [E^n - E^{n-1}] + \Delta t \frac{(e')^n}{e^n} E^n \leq 0$$

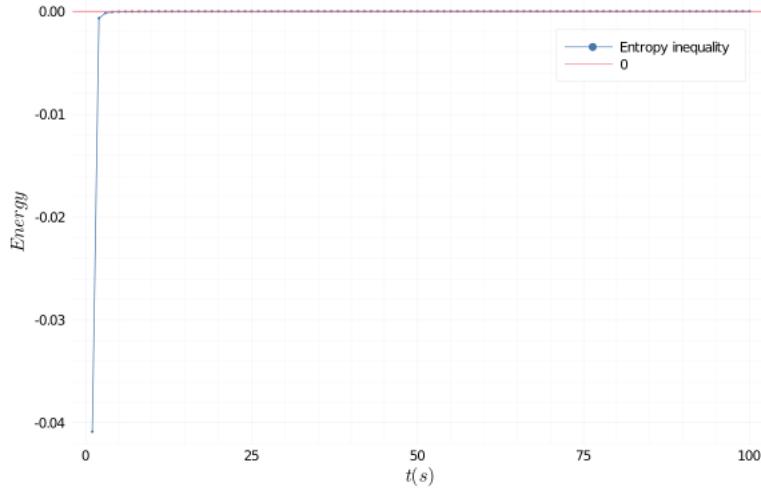


Figure 7: Entropy Inequality

Figure (7.3) shows that the previous inequality is correct for this scheme. In addition, we plotted the Entropy's evolution in Figure (7.3), thought its behaviour was not numerically explained in non-zero flux settings.

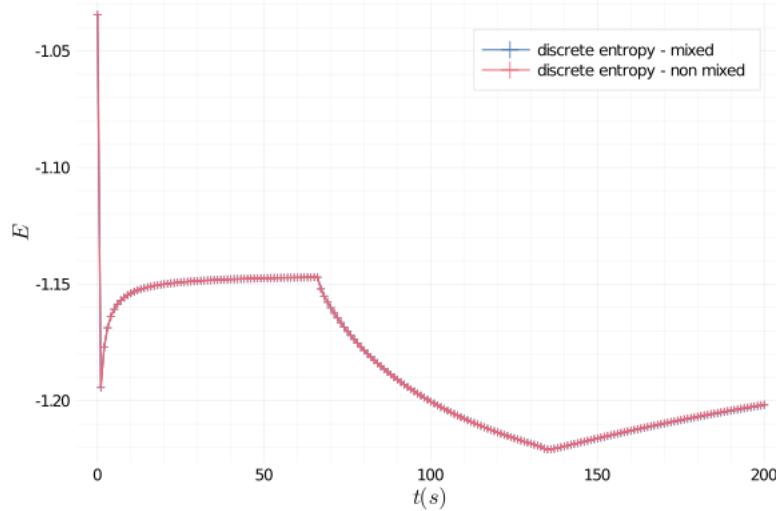


Figure 8: Entropy profile

8 Numerical Simulation : Constant Flux

8.1 Long term profile

We took the parameters displayed in Table (2) for simulating the constant flux behaviour, the latter being depicted in Figure (8.1).

N	4
N_T	10 000
Δt	10
N_d	50
Δx	0.02

Table 2: Discretization Parameters - constant fluxes



Figure 9: Flux

To illustrate the convergence towards the relative fluxes, we chose a different initial profile, as illustrated in Figure (8.1), which shows more pronounced variations as before.

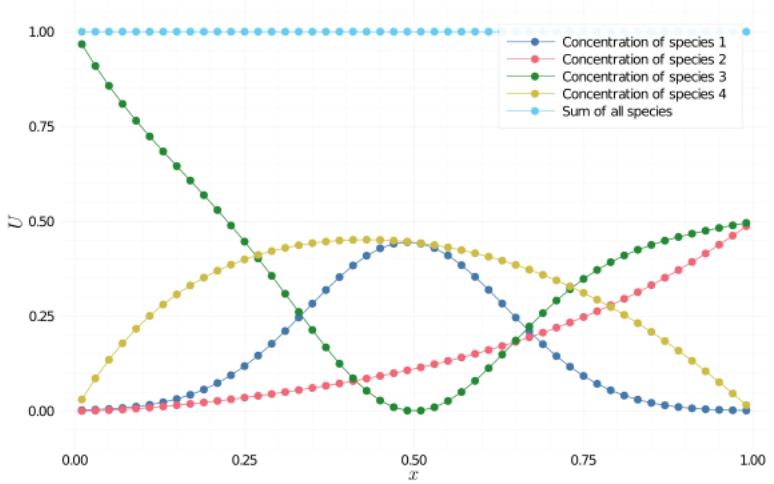


Figure 10: Initial Profile

The result after a thousand iterations is shown below in Figure (8.1), similar to the normalized fluxes above.

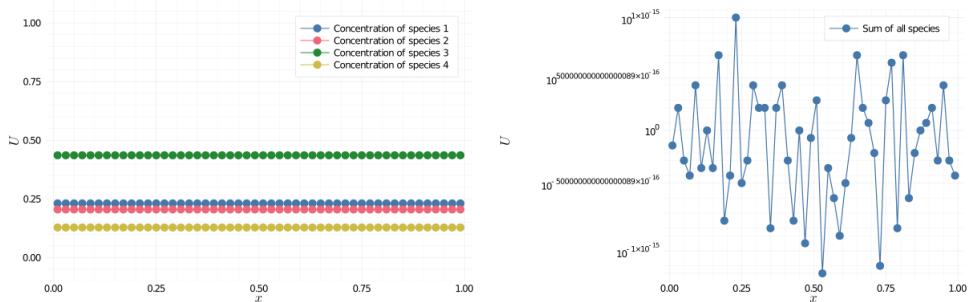


Figure 11: Final Profile

We still have good stability for the space \mathcal{A} . Figure (8.1) shows the difference between the relative flux and the final profile being in the magnitude of 10^{-5} .

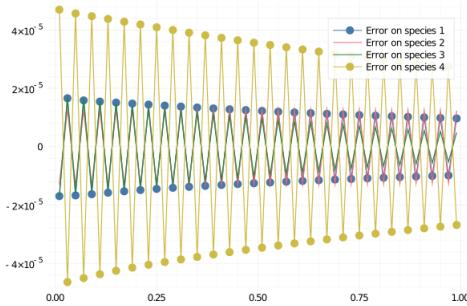


Figure 12: Error between Final Profile and Relative Flux

The mass conservation error is also depicted below in Figure (8.1). Although a spike of 10^{-9} at around $t = 1000s$, the error is quite low.

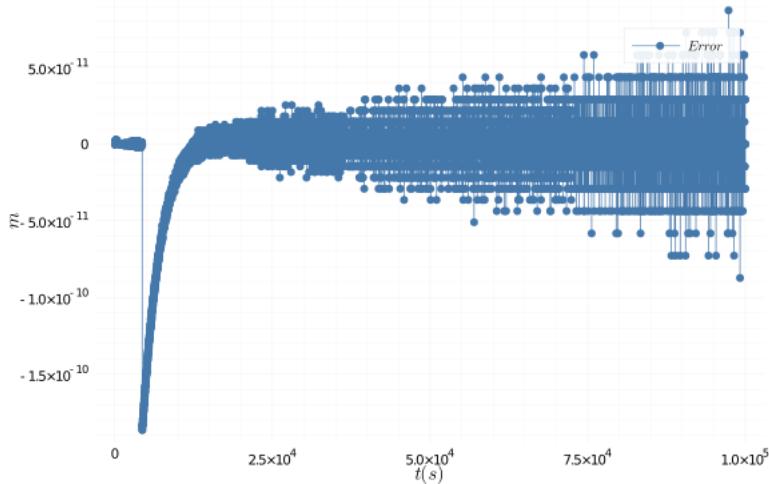


Figure 13: Mass error

Finally, Figure (8.1) is present to confirm the convergence rate depicted in Equation (??). An interesting behavior arise: it seems that before reaching the asymptotic behavior, the convergence slows down.

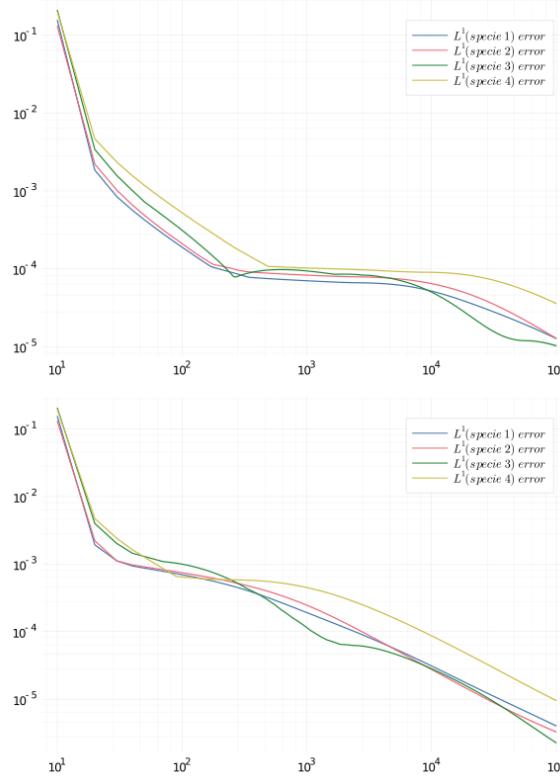


Figure 14: L^1 -error between final profile and target normalized fluxes : (Left) $\Delta x = 0.02$, (Right) $\Delta x = 0.1$ - xaxis : $t(s)$

This behavior can be seen when looking at the "standard deviation" from the mean $\|v_i - \bar{v}_i\|_{L^1}^2$ and the upper bound given from the Csizar-Kullback inequality in

Equation 16, as depicted in Figure (8.1)

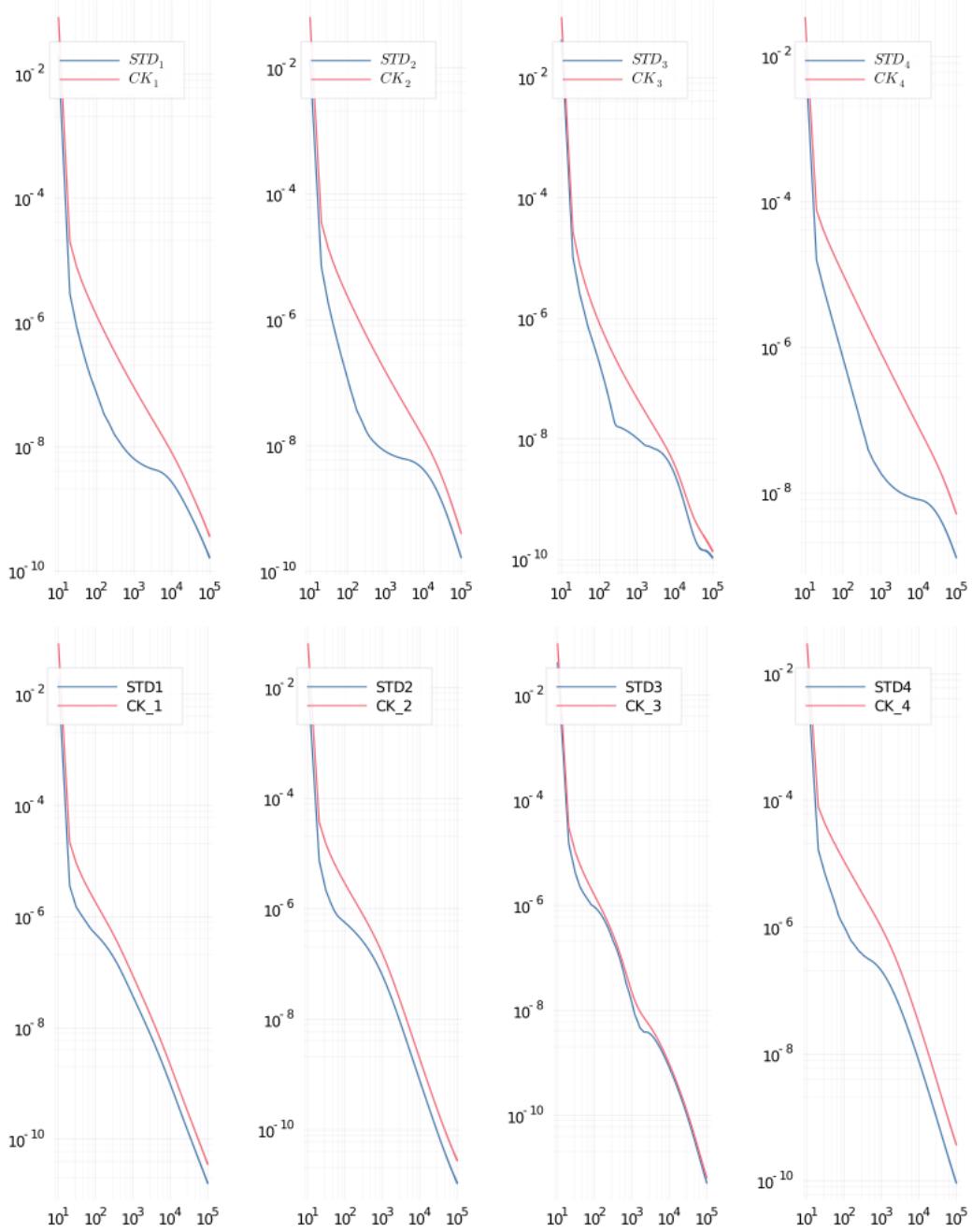


Figure 15: Csizar-Kullback inequality: (Above) $\Delta x = 0.02$, (Below) $\Delta x = 0.1$ - xaxis : $t(s)$

8.2 Entropy

Lastly, the modified entropy inequality of Equation (15) is illustrated in Figure (8.2). This inequality is not sharp as shown in the previous sections (a strict convexity inequality and two other negative terms were omitted in the upper bound).

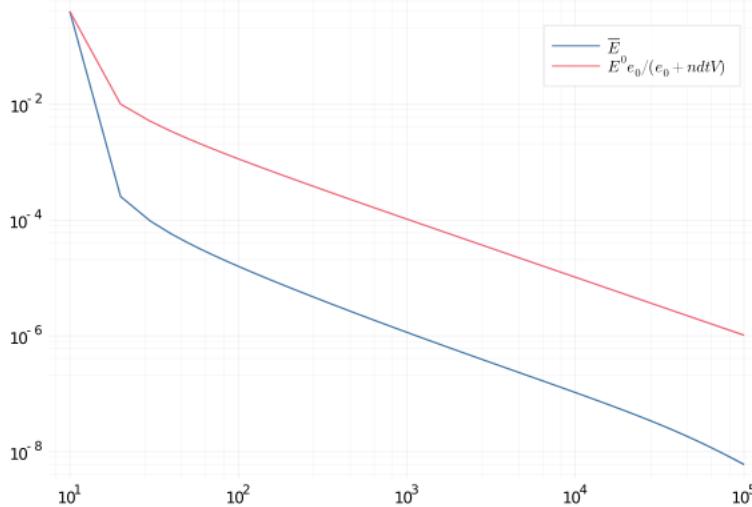


Figure 16: Modified Entropy inequality

Conclusion

Though the problem that we focused on was presented and well-posed in [1], the numerical simulation were done with a scheme that was not converging, due to the addition of fluxes at one end of the one-dimensional model. Preserving key properties from the continuous to the discrete model was key to ensure convergence: hence the *boundedness by entropy* method needed to be adapted [2].

Indeed, having a Lyapunov entropy functional allowed us to have a compactness of the discrete gradient, essential for passing to the limit while proving convergence of our scheme. The boundedness by entropy method worked on the continuous model mainly because of the chain rule linking natural derivative to logarithmic derivative, so in adapting the same property to the numerical scheme we ensured that this property transferred to the discrete model.

To design a numerical scheme that satisfies both the physical properties of concentrations (i.e. positive summing to one) and mass conservation, we needed to use a hybrid implicit/explicit scheme by looking at the drift term and diffusion term separately. While using a Finite Volume scheme was natural due to the physical interpretation of the model (itself deriving from conservation laws), a close inspection of the edge value approximation was made to ensure that all of the aforementioned properties still hold. This is why we made such complex approximations as described in Section 2.

In addition, echoing [1], we also looked at the case of constant fluxes due to the explicit convergence, and we used numerical simulation with the same parameters for better comparison, which illustrated the different theoretical bounds and results accurately.

References

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