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A NUMERICAL ANALYSIS FOCUSED COMPARISON OF SEVERAL FINITE VOLUME SCHEMES FOR AN UNIPOLAR DEGENERATED DRIFT-DIFFUSION MODEL

CLÉMENT CANCÈS, CLAIRE CHAINAIS-HILLAIRET, JÜRGEN FUHRMANN,
AND BENOÎT GAUDEUL

ABSTRACT. In this paper, we consider an unipolar degenerated drift-diffusion system where the relation between the concentration of the charged species c and the chemical potential h is $h(c) = \log \frac{c}{1-c}$. We design four different finite volume schemes based on four different formulations of the fluxes. We provide a stability analysis and existence results for the four schemes. The convergence proof with respect to the discretization parameters is established for two of them. Numerical experiments illustrate the behaviour of the different schemes.

1. INTRODUCTION

1.1. **Motivation.** Unipolar drift-diffusion models describe the transport of a charged species in the presence of a fixed or moving countercharge. They consist of the coupling of a drift-diffusion equation on the density of the charged species c with a Poisson equation on the electric potential Φ . They can be written under a general form as

$$\begin{cases} \partial_t c + \operatorname{div}(\mathbf{J}) = 0, & \mathbf{J} = -\eta(c)\nabla(h(c) + \Phi), \\ -\lambda^2 \Delta \Phi = c + c^{dp}, \end{cases}$$

where h is the chemical potential, η the mobility coefficient, λ the scaled Debye length coming from the nondimensionalization of the physical model and c^{dp} describes the doping profile of the media.

Such models occur in a number of interesting application cases. Charge carriers in most classical semiconductors exhibit a relationship $c = \mathcal{F}(h)$, where \mathcal{F} is the Fermi integral of index $\frac{1}{2}$ which can be approximated in the range $-\infty < h \lesssim 1.3$ by the function $\mathcal{F}(h) = \frac{1}{\gamma + \exp(-h)}$ with $\gamma = 0.27$ [6]. For $\gamma = 1$, this relationship corresponds to the Fermi integral of index -1 and implies $h = \log \frac{c}{1-c}$. It is the limit for vanishing disorder of the Gauss-Fermi integral [37, 39] which is used to describe organic semiconductors [15]. A similar relationship is valid for the oxygen ion concentration in a solid oxide electrolyte [43] and in a simple model of an ionic liquid [28].

While the relationship between chemical potential and concentration is sufficient to describe the thermodynamic equilibrium, the description of charge transport driven by the sum of the gradients of the chemical potential and the electrostatic potential Φ needs an additional specification of the mobility coefficient η . Setting this coefficient proportional to the concentration c is common in the case of semiconductors [42]. A similar ansatz describes the limit of large lattice mass density in solid oxide electrolytes. It also follows from a formal reduction of an generalized Nernst-Planck model [19, 18] to the case of a mixture of two charged species including an infinitely mobile and charged solvent – ionic liquids – as performed in [28]. We hint that more general and fully consistent models for both solid oxide electrolytes and ionic liquids consider mobility coefficients of the type $c(1-c)$ [43, 8, 33].

In this paper, we consider that the mobility coefficient is $\eta(c) = c$ and the chemical potential $h(c) = \log \frac{c}{1-c}$ (corresponding to $\mathcal{F}(h) = \frac{1}{1+\exp(-h)}$). Strong degeneration described by a bounded dependency of the concentration c on the chemical potential h leads to a number of structural mathematical challenges in the corresponding drift-diffusion models. These need to be addressed properly in numerical schemes. The consideration of this simplified model is a starting point for the study of generalized Nernst-Planck models for multiple ionic species in electroneutral solvents [19, 18, 27, 28]. Moreover, the design of discretization methods for the case where $\eta(c) = c(1-c)$ is also possible topic of further investigation following the present paper.

1.2. A simplified unipolar degenerate drift-diffusion model. Let us now define the framework of the study. We consider the evolution of a the concentration c of a charged species in a connected bounded open domain Ω of \mathbb{R}^d ($d \leq 3$) with polyhedral and Lipschitz continuous boundary $\partial\Omega$ during a finite but arbitrary time $T > 0$. After nondimensionalization with appropriate scaling, we regard the following system of partial differential equations (PDEs). The concentration c satisfies the conservation law

$$\partial_t c + \operatorname{div}(\mathbf{J}) = 0 \quad \text{in } (0, T) \times \Omega. \quad (1.1)$$

The flux \mathbf{J} is negatively proportional to the gradient of the electrochemical potential as expressed by the expression

$$\mathbf{J} = -c\nabla(h(c) + \Phi) \quad \text{in } (0, T) \times \Omega, \quad (1.2)$$

where $h(c) = \log\left(\frac{c}{1-c}\right)$ is the chemical potential. In what follows, we consider that the electrostatic potential Φ is related to space charge density thanks to the Poisson equation

$$-\Delta\Phi = c + c^{dp} \quad \text{in } (0, T) \times \Omega, \quad (1.3)$$

which means that the Debye length is set to 1. Extension to general Debye length is straightforward. The doping profile c^{dp} is assumed to be constant w.r.t. time and to be bounded, i.e., $c^{dp} \in L^\infty(\Omega)$.

One interpretation of c is the concentration of majority carriers (holes) in a p-type organic semiconductor with constant in time doping. Another interpretation of c is the cation concentration in an ionic liquid following the formal approach introduced in [28].

The system is supplemented with the prescription of the initial concentration

$$c|_{t=0} = c^0 \in L^\infty(\Omega) \quad \text{with} \quad 0 \leq c^0 \leq 1 \quad \text{and} \quad 0 < \bar{c} = \int_{\Omega} c^0 d\mathbf{x} < 1, \quad (1.4)$$

and of boundary conditions. The choice of the boundary conditions may depend on the targeted application: organic semiconductor or ionic liquid. For the analysis purpose, we consider boundary conditions which are well adapted to the ionic liquid model. Other boundary conditions will also be considered in the numerical simulations in Section 5. There are no-flux boundary conditions for the concentration:

$$\mathbf{J} \cdot \mathbf{n} = 0 \quad \text{on } (0, T) \times \partial\Omega. \quad (1.5)$$

And concerning the Poisson equation (1.3), it is supplemented with inhomogeneous Dirichlet boundary conditions on a part Γ_D of $\partial\Omega$, and by homogeneous Neumann boundary condition on the remaining part $\Gamma_N = \partial\Omega \setminus \Gamma_D$ of the boundary:

$$\Phi = \Phi^D \quad \text{on } (0, T) \times \Gamma_D, \quad \nabla\Phi \cdot \mathbf{n} = 0 \quad \text{on } (0, T) \times \Gamma_N. \quad (1.6)$$

Throughout the paper, we assume that Φ^D is defined on the whole domain Ω and does not depend on time, with $\Phi^D \in H^1(\Omega) \cap L^\infty(\Omega)$.

The goal of this paper is to study and compare several different Finite Volume schemes for the system (1.1)–(1.6). They are based on various reformulations of the flux \mathbf{J} . Indeed,

we may introduce either the so-called excess chemical potential $\nu(c) = h(c) - \log(c) = -\log(1-c)$, or the activity and the inverse activity coefficient respectively defined by $a(c) = e^{h(c)} = \frac{c}{1-c}$, and $\beta(c) = \frac{c}{a(c)} = 1-c$, or the diffusion enhancement $r(c) = -\log(1-c)$ satisfying $r'(c) = ch'(c)$. Then the flux \mathbf{J} , initially defined by (1.2), rewrites

$$\mathbf{J} = -\nabla c - c\nabla(\Phi + \nu(c)), \quad (1.7)$$

$$= -\beta(c)(\nabla a(c) + a(c)\nabla\Phi), \quad (1.8)$$

$$= -r'(c)\nabla c - c\nabla\Phi, \quad (1.9)$$

These formulations (1.2), (1.7), (1.8) and (1.9) lead to different schemes that we aim to compare from a numerical analysis point of view. We may notice that the flux \mathbf{J} also rewrites

$$\mathbf{J} = -\nabla r(c) - c\nabla\Phi. \quad (1.10)$$

This last formulation will be used to define the weak solution to (1.1)–(1.6).

Before going to the discretization of the problem, let us highlight the entropy structure of system (1.1)–(1.6), which plays a central role in what follows.

1.3. Entropy structure and weak solutions. The goal of this section is to shortly depict the gradient flow structure of the system (1.1)–(1.6). We stay here at a formal level, and remain sloppy about regularity issues. The solutions (c, Φ) to (1.1)–(1.6) are supposed to be regular enough so that the following calculations are justified. Define the mixing entropy density

$$H(c) = c \log(c) + (1-c) \log(1-c),$$

which is an antiderivative of h , then the electrochemical energy is given by

$$E(c, \Phi) = \int_{\Omega} \left\{ H(c) + \frac{1}{2} |\nabla\Phi|^2 \right\} d\mathbf{x} - \int_{\Gamma_D} \Phi^D \nabla\Phi \cdot \mathbf{n} d\gamma. \quad (1.11)$$

The next proposition shows that the electrochemical energy is a Lyapunov functional. Moreover, the dissipation rate for the energy is explicitly given.

prop:E

Proposition 1.1. *Let (c, Φ) be a smooth solution to (1.1)–(1.6), with c bounded away from 0 and 1, then*

$$\frac{d}{dt} E(c, \Phi) + \int_{\Omega} c |\nabla(h(c) + \Phi)|^2 d\mathbf{x} = 0.$$

Proof. We notice first that, since Φ^D does not depend on time,

$$\frac{d}{dt} E(c, \Phi) = \int_{\Omega} (h(c) \partial_t c + \nabla\Phi \cdot \partial_t \nabla\Phi) d\mathbf{x} - \int_{\Gamma_D} \Phi^D \partial_t \nabla\Phi \cdot \mathbf{n} d\gamma.$$

Then we apply the Gauss theorem and we use the Poisson equation (1.3) with a constant doping profile, in order to get

$$\frac{d}{dt} E(c, \Phi) = \int_{\Omega} (h(c) + \Phi) \partial_t c.$$

Multiplying the conservation law (1.1) by $h(c) + \Phi$ and integrating over the domain Ω yields

$$\int_{\Omega} \partial_t c (h(c) + \Phi) = - \int_{\Omega} c |\nabla(h(c) + \Phi)|^2 d\mathbf{x},$$

thanks to the no-flux boundary condition (1.5). It concludes the proof of Proposition 1.1. \square

{Sedan flu

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{Weak solu

{eq:E}

Let $c \in L^\infty(\Omega; [0, 1])$, we denote by $\Phi[c]$ the unique solution to (1.3). One can easily check that the energy functional $c \mapsto E(c, \Phi[c])$ is bounded on $L^\infty(\Omega; [0, 1])$. Indeed, H takes values in $[-\log 2, 0]$ and the bounds on the electrical energy can be obtained by multiplying the Poisson equation by $\Phi - \Phi^D$ and Φ and integrating over Ω . Therefore, $E(c(t), \Phi(t))$ is finite for all $t > 0$, whence a $L^\infty((0, T); H^1(\Omega))$ estimate on Φ . We also deduce from Proposition 1.1 that the total energy dissipation is bounded, i.e.

$$\int_0^T \int_\Omega c |\nabla(h(c) + \Phi)|^2 d\mathbf{x} dt \leq C \quad (1.12) \quad \boxed{\text{eq:dissip}}$$

for some C uniform with respect to the final time horizon T . Using again that $0 \leq c \leq 1$, we deduce from (1.12) that

$$\int_0^T \int_\Omega |\nabla r(c)|^2 d\mathbf{x} dt \leq \int_0^T \int_\Omega c |\nabla h(c)|^2 d\mathbf{x} dt \leq C. \quad (1.13) \quad \boxed{\text{eq:L2H1_r}}$$

The aforementioned $L^\infty((0, T); H^1(\Omega))$ estimate on the potential Φ and Estimate (1.13) on $r(c)$ suggest a notion of weak solution which is based on the expression (1.10) of the flux \mathbf{J} . In what follows, we denote the vector space $\mathcal{H}_{\Gamma^D} = \{f \in H^1(\Omega), f_{\Gamma^D} = 0\}$ and $Q_T = (0, T) \times \Omega$.

Definition 1. A couple (c, Φ) is a weak solution of (1.1)–(1.6) if

- $c \in L^\infty((0, T); [0, 1])$ with $r(c) \in L^2((0, T); H^1(\Omega))$, and $\Phi - \Phi^D \in L^\infty((0, T), \mathcal{H}_{\Gamma^D})$;
- For all $\varphi \in C_c^\infty([0, T) \times \bar{\Omega})$, there holds

$$\iint_{Q_T} c \partial_t \varphi d\mathbf{x} dt + \int_\Omega c^0 \varphi(0, \cdot) d\mathbf{x} - \iint_{Q_T} (r(c) + c \nabla \Phi) \cdot \nabla \varphi d\mathbf{x} dt = 0; \quad (1.14) \quad \boxed{\text{eq:weak_c}}$$

- For all $\psi \in \mathcal{H}$ and almost all $t \in (0, T)$, there holds

$$\int_\Omega \nabla \Phi(t, \mathbf{x}) \cdot \nabla \psi(\mathbf{x}) d\mathbf{x} = \int_\Omega (c(t, \mathbf{x}) + c^{dp}(\mathbf{x})) \psi(\mathbf{x}) d\mathbf{x}. \quad (1.15) \quad \boxed{\text{eq:weak_P}}$$

The goal of this paper is to compare from a numerical analysis point of view several different numerical schemes to approximate the solutions to (1.1)–(1.6). We pay a particular attention to the preservation at the discrete level of the key properties of the continuous model, in particular concerning the preservation of the physical bounds $0 \leq c \leq 1$ and the energy/energy dissipation relation highlighted in Proposition 1.1. The definition of the Finite Volume approximation is detailed in the next section.

2. FINITE VOLUME APPROXIMATIONS

This section is organized as follows. First in Section 2.1, we state the requirements on the mesh and fix some notations. Then in Section 2.2, we describe the common basis to the different schemes to be studied in this paper. All the methods presented in this paper rely on so-called two-point flux approximations, but four different schemes are introduced in Section 2.3 based on the formulations (1.2) to (1.9) of the flux \mathbf{J} . Then in Section 2.4, we state our two main results. The first one, namely Theorem 2.1, focuses on the case of a fixed mesh. We are interested in the existence of a solution to the nonlinear system corresponding to the schemes, and to the dissipation of the energy at the discrete level. More precisely, one establishes that the all the studied schemes satisfy a discrete counterpart to Proposition 1.1. Our second main result, namely Theorem 2.2, is devoted to the convergence of the scheme as the time step and the mesh size tend to 0.

ssec:mesh

2.1. **Discretization of $(0, T) \times \Omega$.** In this paper, we perform a parallel study of four numerical schemes based on two-point flux approximation (TPFA) finite volume schemes. As explained in [20, 24], this approach appears to be very efficient as soon as the continuous problem to be solved numerically are isotropic and one has the freedom to choose a suitable mesh fulfilling the so-called orthogonality condition [36, 25]. We recall here the definition of such a mesh, which is illustrated by Figure 1.

def:mesh

Definition 2. An admissible mesh of Ω is a triplet $(\mathcal{T}, \mathcal{E}, (\mathbf{x}_K)_{K \in \mathcal{T}})$ such that the following conditions are fulfilled.

- (i) Each control volume (or cell) $K \in \mathcal{T}$ is non-empty, open, polyhedral and convex. We assume that

$$K \cap L = \emptyset \quad \text{if } K, L \in \mathcal{T} \text{ with } K \neq L, \quad \text{while} \quad \bigcup_{K \in \mathcal{T}} \bar{K} = \bar{\Omega}.$$

- (ii) Each face $\sigma \in \mathcal{E}$ is closed and is contained in a hyperplane of \mathbb{R}^d , with positive $(d-1)$ -dimensional Hausdorff (or Lebesgue) measure denoted by $m_\sigma = \mathcal{H}^{d-1}(\sigma) > 0$. We assume that $\mathcal{H}^{d-1}(\sigma \cap \sigma') = 0$ for $\sigma, \sigma' \in \mathcal{E}$ unless $\sigma' = \sigma$. For all $K \in \mathcal{T}$, we assume that there exists a subset \mathcal{E}_K of \mathcal{E} such that $\partial K = \bigcup_{\sigma \in \mathcal{E}_K} \sigma$. Moreover, we suppose that $\bigcup_{K \in \mathcal{T}} \mathcal{E}_K = \mathcal{E}$. Given two distinct control volumes $K, L \in \mathcal{T}$, the intersection $\bar{K} \cap \bar{L}$ either reduces to a single face $\sigma \in \mathcal{E}$ denoted by $K|L$, or its $(d-1)$ -dimensional Hausdorff measure is 0.
- (iii) The cell-centers $(\mathbf{x}_K)_{K \in \mathcal{T}}$ are pairwise distinct with $\mathbf{x}_K \in K$, and are such that, if $K, L \in \mathcal{T}$ share a face $K|L$, then the vector $\mathbf{x}_L - \mathbf{x}_K$ is orthogonal to $K|L$.
- (iv) For the boundary faces $\sigma \subset \partial\Omega$, we assume that either $\sigma \subset \Gamma_D$ or $\sigma \subset \bar{\Gamma}_N$. For $\sigma \subset \partial\Omega$ with $\sigma \in \mathcal{E}_K$ for some $K \in \mathcal{T}$, we assume additionally that there exists $\mathbf{x}_\sigma \in \sigma$ such that $\mathbf{x}_\sigma - \mathbf{x}_K$ is orthogonal to σ .

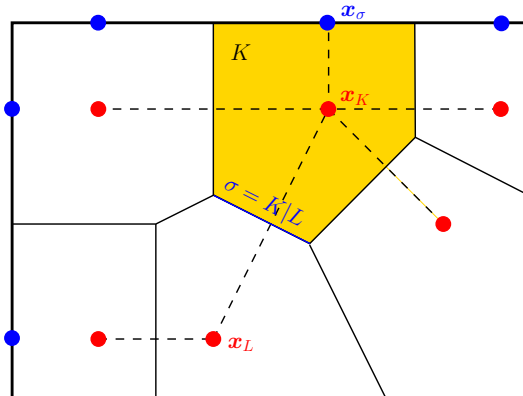


FIGURE 1. Illustration of an admissible mesh as in Definition 2.

fig:mesh

We denote by m_K the d -dimensional Lebesgue measure of the control volume K . The set of the faces is partitioned into two subsets: the set \mathcal{E}_{int} of the interior faces defined by $\mathcal{E}_{\text{int}} = \{\sigma \in \mathcal{E} \mid \sigma = K|L \text{ for some } K, L \in \mathcal{T}\}$, and the set \mathcal{E}_{ext} of the exterior faces defined by $\mathcal{E}_{\text{ext}} = \{\sigma \in \mathcal{E} \mid \sigma \subset \partial\Omega\}$, which can also be partitioned into $\mathcal{E}^D = \{\sigma \subset \Gamma_D\}$ and $\mathcal{E}^N = \{\sigma \subset \bar{\Gamma}_N\}$. For a given control volume $K \in \mathcal{T}$, we also define $\mathcal{E}_{K,\text{int}}$ the set of its faces which belong to \mathcal{E}_{int} . For such a face $\sigma \in \mathcal{E}_{K,\text{int}}$, we may write $\sigma = K|L$, meaning that $\sigma = \bar{K} \cap \bar{L}$.

Given $\sigma \in \mathcal{E}$, we denote by

$$d_\sigma = \begin{cases} |\mathbf{x}_K - \mathbf{x}_L| & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int}}, \\ |\mathbf{x}_K - \mathbf{x}_\sigma| & \text{if } \sigma \in \mathcal{E}_{\text{ext}}, \end{cases} \quad \text{and by } \tau_\sigma = \frac{m_\sigma}{d_\sigma}$$

We finally introduce the size $h_\mathcal{T}$ and the regularity $\zeta_\mathcal{T}$ (which is assumed to be positive) of a discretization $(\mathcal{T}, \mathcal{E}, (\mathbf{x}_K)_{K \in \mathcal{T}})$ of Ω by setting

$$h_\mathcal{T} = \max_{K \in \mathcal{T}} \text{diam}(K), \quad \zeta_\mathcal{T} = \min_{K \in \mathcal{T}} \min_{\sigma \in \mathcal{E}_K} \frac{d(\mathbf{x}_K, \sigma)}{d_\sigma}.$$

Concerning the time discretization of $(0, T)$, we consider an increasing finite family of times $0 = t_0 < t_1 < \dots < t_N = T$. We denote by $\Delta t_n = t_n - t_{n-1}$ for $1 \leq n \leq N$, by $\mathbf{\Delta t} = (\Delta t_n)_{1 \leq n \leq N}$, and by $\overline{\mathbf{\Delta t}} = \max_{1 \leq n \leq N} \Delta t_n$.

sec:scheme

2.2. A common basis for the Finite Volume schemes. All the numerical schemes studied in this paper are based on TPFA Finite Volumes. The initial data c_0 is discretized into $(c_K^0)_{K \in \mathcal{T}} \in \mathbb{R}^\mathcal{T}$ by setting

$$c_K^0 = \frac{1}{m_K} \int_K c^0(\mathbf{x}) d\mathbf{x}, \quad \forall K \in \mathcal{T}, \quad \{\text{eq:cK0}\}$$

while the doping profile c^{dp} is discretized into $(c_K^{dp})_{K \in \mathcal{T}} \in \mathbb{R}^\mathcal{T}$ by

$$c_K^{dp} = \frac{1}{m_K} \int_K c^{dp}(\mathbf{x}) d\mathbf{x}, \quad \forall K \in \mathcal{T}. \quad \{\text{eq:cKdp}\}$$

Assume that $\mathbf{c}^{n-1} = (c_K^{n-1})_{K \in \mathcal{T}}$ is given for some $n > 0$, then we have to define how to compute $(\mathbf{c}^n, \mathbf{\Phi}^n) = (c_K^n, \Phi_K^n)_{K \in \mathcal{T}}$.

First, we introduce some notations. For all $K \in \mathcal{T}$ and all $\sigma \in \mathcal{E}_K$, we define the mirror values $c_{K\sigma}^n$ and $\Phi_{K\sigma}^n$ of c_K^n and Φ_K^n respectively across σ by setting

$$c_{K\sigma}^n = \begin{cases} c_L^n & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int}}, \\ c_K^n & \text{if } \sigma \in \mathcal{E}_{\text{ext}}, \end{cases} \quad \Phi_{K\sigma}^n = \begin{cases} \Phi_L^n & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int}}, \\ \Phi_K^n & \text{if } \sigma \in \mathcal{E}^N, \\ \Phi_\sigma^n = \frac{1}{m_\sigma} \int_\sigma \Phi^D d\gamma & \text{if } \sigma \in \mathcal{E}^D. \end{cases} \quad \{\text{eq:mirror}\}$$

Given $\mathbf{u} = (u_K)_{K \in \mathcal{T}} \in \mathbb{R}^\mathcal{T}$, we define the oriented and absolute jumps of \mathbf{u} across any edge by

$$D_{K\sigma} \mathbf{u} = u_{K\sigma} - u_K, \quad D_\sigma \mathbf{u} = |D_{K\sigma} \mathbf{u}|, \quad \forall K \in \mathcal{T}, \forall \sigma \in \mathcal{E}_K.$$

We consider a backward Euler scheme in time and a TPFA finite volume scheme in space. It is written as follows:

scheme

$$-\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K\sigma} \mathbf{\Phi}^n = m_K (c_K^n + c_K^{dp}), \quad \forall K \in \mathcal{T}. \quad \{\text{eq:scheme}\}$$

$$m_K \frac{c_K^n - c_K^{n-1}}{\Delta t_n} + \sum_{\sigma \in \mathcal{E}_K} F_{K\sigma}^n = 0, \quad \forall K \in \mathcal{T}, \quad \{\text{eq:scheme}\}$$

where $F_{K\sigma}^n$ should be a conservative and consistent approximation of $\frac{1}{\Delta t_n} \int_{t_{n-1}}^{t_n} \int_\sigma \mathbf{J} \cdot \mathbf{n}_{K\sigma}$ ($\mathbf{n}_{K\sigma}$ denotes the normal to σ outward K). The explicit formulas relating the numerical fluxes $F_{K\sigma}^n$ to the primary unknowns are now the only remaining degree of freedom. Four possible choices are given in the next section.

sec:fluxes

2.3. Numerical fluxes for the conservation of the chemical species. In order to close the system (2.4a)–(2.4b), it remains to define the numerical fluxes $F_{K\sigma}^n$.

Due to the no-flux boundary condition (1.5), we impose, in all the cases,

$$F_{K\sigma}^n = 0, \quad \forall K \in \mathcal{T}, \forall \sigma \in \mathcal{E}_K \cap \mathcal{E}_{\text{ext}}. \quad (2.5)$$

{eq:noflux

The inner fluxes are defined with a function \mathcal{F} of the primary unknowns $(c_K^n, c_L^n, \Phi_K^n, \Phi_L^n)$:

$$F_{K\sigma}^n = \tau_\sigma \mathcal{F}(c_K^n, c_L^n, \Phi_K^n, \Phi_L^n), \quad \forall K \in \mathcal{T}, \forall \sigma = K|L. \quad (2.6)$$

{eq:fluxin

We discuss now four strategies that are based on the four expressions (1.2), (1.7), (1.8), and (1.9). They lead to different formulas for \mathcal{F} . Three of the discrete fluxes are extensions of the Scharfetter-Gummel scheme [41] and let the Bernoulli function $B(u) = \frac{u}{e^u - 1}$, with $B(0) = 1$, appear in their definition.

All the functions \mathcal{F} defined below verify

$$\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) = -\mathcal{F}(c_L, c_K, \Phi_L, \Phi_K) \quad \forall (c_K, c_L, \Phi_K, \Phi_L) \in (0, 1) \times (0, 1) \times \mathbb{R} \times \mathbb{R},$$

so that the numerical fluxes are locally conservative, which means

$$F_{K\sigma}^n + F_{L\sigma}^n = 0 \quad \forall \sigma = K|L \in \mathcal{E}_{\text{int}}. \quad (2.7)$$

{eq:cons_F

c:centered

2.3.1. The centered flux. The so-called centered flux is derived from formula (1.2), which suggests the following definition of \mathcal{F} :

$$\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) = -\frac{c_K + c_L}{2} D_{K\sigma} (h(\mathbf{c}) + \Phi). \quad (2.8)$$

{eq:center

The associate flux can be seen as a particular case in the TPFA context of the fluxes introduced in [12, 10, 9, 13] in various multipoint flux approximations (MPFA) or finite element contexts. In opposition to the three next schemes, the centered scheme is not based on the Scharfetter-Gummel scheme. We can notice that, even if the relation (1.10) between the flux and the concentration would be linear (i.e., if $h(c) = \log(c)$ so that $r(c) = c$), \mathcal{F} is nonlinear with respect to c_K and c_L and also singular near 0.

ssec:Sedan

2.3.2. The Sedan flux. The second flux we introduce is named Sedan after the eponymous code SEDAN III [44]. Formula (1.7) for the flux \mathbf{J} suggests to use a classical Scharfetter-Gummel scheme, but for a modified potential $\Phi + \nu(c)$ instead of only Φ , leading to the following definition of \mathcal{F} :

$$\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) = \left\{ B(D_{K\sigma}(\Phi + \nu(\mathbf{c}))) c_K - B(-D_{K\sigma}(\Phi + \nu(\mathbf{c}))) c_L \right\}. \quad (2.9)$$

{eq:SEDAN_

rem:Sedan

Remark 2.1. We notice that the Sedan flux defined by (2.9) satisfies

$$\mathcal{F}(c_K, c_L, \Phi, \Phi) = r(c_K) - r(c_L), \quad \forall (c_K, c_L) \in (0, 1) \times (0, 1), \quad \forall \Phi \in \mathbb{R}.$$

It means that, when $\mathbf{J} = -\nabla r(c)$, we recover the classical two-point flux approximation:

$$F_{K\sigma}^n = \tau_\sigma (r(c_K^n) - r(c_L^n)), \quad \forall K \in \mathcal{T}, \forall \sigma = K|L.$$

c:activity

2.3.3. *The activity based flux.* The activity based flux we discuss now is a restriction to our simplified model of the flux introduced in [27, 31]. It relies on the expression (1.8) of the flux \mathbf{J} . Assume that $a(c)$ and $\beta(c)$ are independent one from another (even though this is of course not true), then the flux \mathbf{J} is linear w.r.t. $a(c)$, while $\beta(c)$ is a multiplicative factor. This suggests to choose a particular average for $\beta(c)$ —here the arithmetic mean—and to apply the Scharfetter-Gummel scheme in order to approximate $\nabla a(c) + a(c)\nabla\Phi$. This yields

$$\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) = \frac{\beta(c_K) + \beta(c_L)}{2} \left\{ B(D_{K\sigma}\Phi)a(c_K) - B(-D_{K\sigma}\Phi)a(c_L) \right\}. \quad (2.10)$$

{eq:activi

s:Marianne

2.3.4. *The Bessemoulin-Chatard flux.* The last numerical flux we consider here is named Bessemoulin-Chatard flux after the author's name of [3]. Formula (1.9) for the flux \mathbf{J} suggests that, up to the introduction of a variable diffusion coefficient approximating the quantity $r'(c)$ per face, one can use the Scharfetter-Gummel scheme. Following [3], the approximation $dr(c_K, c_L)$ of $r'(c)$ is defined as

$$dr(c_K, c_L) = \begin{cases} \frac{h(c_K) - h(c_L)}{\log(c_K) - \log(c_L)} & \text{if } c_K \neq c_L, \\ r'(c_K) & \text{if } c_K = c_L. \end{cases}$$

This leads to the following definition of \mathcal{F} :

$$\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) = dr(c_K, c_L) \left\{ B\left(\frac{D_{K\sigma}\Phi}{dr(c_K, c_L)}\right) c_K - B\left(-\frac{D_{K\sigma}\Phi}{dr(c_K, c_L)}\right) c_L \right\}. \quad (2.11)$$

{eq:Marian

ssec:main

2.4. **Main results and organisation of the paper.** We have introduced four schemes defined by (2.1)–(2.6), supplemented with one of the four definitions of \mathcal{F} : (2.8), (2.9), (2.10), or (2.11). Besides numerical comparisons between the different approaches—this will be the purpose of Section 5—, we aim at proposing shared pieces of numerical analysis for all the schemes.

All the four schemes proposed above yield a nonlinear system to be solved at each time step. The first theorem proven in this paper concerns the existence of discrete solutions for a given mesh, and the preservation of the physical bounds: boundedness of the concentration between 0 and 1, decay of the energy. The discrete energy functional $E_{\mathcal{T}}$ is the discrete counterpart of the continuous energy functional E , namely

$$E_{\mathcal{T}}(\mathbf{c}^n, \Phi^n) = \sum_{K \in \mathcal{T}} m_K H(c_K^n) + \frac{1}{2} \sum_{\sigma \in \mathcal{E}} \tau_{\sigma} (D_{\sigma}\Phi^n)^2 - \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}^D \cap \mathcal{E}_K} \tau_{\sigma} \Phi_{\sigma}^D D_{K\sigma}\Phi^n. \quad (2.12)$$

{eq:E_T}

As stated in Theorem 2.1 below, the nonlinear systems corresponding to all the four schemes admit solutions which preserve the physical bounds on the concentrations and the decay of the energy. The proof of Theorem 2.1 will be the purpose of Section 3.

thm:main1

Theorem 2.1. *Let $(\mathcal{T}, \mathcal{E}, (\mathbf{x}_K)_{K \in \mathcal{T}})$ be an admissible mesh and let \mathbf{c}^0 be defined by (2.1). Then, for all $1 \leq n \leq N$, the nonlinear system of equations (2.3)–(2.6), supplemented either with (2.8), (2.9), (2.10), or (2.11), has a solution $(\mathbf{c}^n, \Phi^n) \in [0, 1]^{\mathcal{T}} \times \mathbb{R}^{\mathcal{T}}$. Moreover, the solution to the scheme satisfies, for all $1 \leq n \leq N$,*

$$E_{\mathcal{T}}(\mathbf{c}^n, \Phi^n) \leq E_{\mathcal{T}}(\mathbf{c}^{n-1}, \Phi^{n-1}) \text{ and } 0 < c_K^n < 1, \quad \forall K \in \mathcal{T}.$$

Knowing a discrete solution to the scheme, $(\mathbf{c}^n, \Phi^n)_{1 \leq n \leq N}$, we can define an approximate solution $(c_{\mathcal{T}, \Delta t}, \Phi_{\mathcal{T}, \Delta t})$. It is the piecewise constant function defined almost everywhere by

$$c_{\mathcal{T}, \Delta t}(t, \mathbf{x}) = c_K^n, \quad \Phi_{\mathcal{T}, \Delta t}(t, \mathbf{x}) = \Phi_K^n \quad \text{if } (t, \mathbf{x}) \in (t_{n-1}, t_n] \times K.$$

This definition will be developed in Section 4 and supplemented by other reconstruction operators.

Let $(\mathcal{T}_m, \mathcal{E}_m, (\mathbf{x}_K)_{K \in \mathcal{T}_m})_{m \geq 1}$ be a sequence of admissible meshes in the sense of Definition 2 such that $h_{\mathcal{T}_m}, \overline{\Delta \mathbf{t}_m} \xrightarrow{m \rightarrow \infty} 0$ while the mesh regularity remains bounded, i.e., $\zeta_{\mathcal{T}_m} \geq \zeta^*$ for some $\zeta^* > 0$ not depending on m , a natural question is the convergence of the associated sequence of approximate solution $(c_{\mathcal{T}_m, \Delta \mathbf{t}_m}, \Phi_{\mathcal{T}_m, \Delta \mathbf{t}_m})_{m \geq 1}$ towards a weak solution to the continuous problem. The convergence result is stated in Theorem 2.2, only for the centered scheme and the Sedan scheme.

Theorem 2.2. *For the centered scheme (inner fluxes defined by (2.6) and (2.8)) and the Sedan scheme (inner fluxes defined by (2.6) and (2.9)), a sequence of approximate solutions $(c_{\mathcal{T}_m, \Delta \mathbf{t}_m}, \Phi_{\mathcal{T}_m, \Delta \mathbf{t}_m})_{m \geq 1}$ satisfies, up to a subsequence,*

$$c_{\mathcal{T}_m, \Delta \mathbf{t}_m} \xrightarrow{m \rightarrow \infty} c \quad \text{a.e. in } Q_T, \quad \Phi_{\mathcal{T}_m, \Delta \mathbf{t}_m} \xrightarrow{m \rightarrow \infty} \Phi \quad \text{in } L^2(Q_T) \quad (2.13)$$

where (c, Φ) is a weak solution in the sense of Definition 1.

The above theorem deserves some comments. First, the convergence proof carried out in what follows does not encompass the activity based scheme and the Bessemoulin-Chatard scheme for reasons that will appear clearly in the proof later on. This does of course not mean that these schemes do not converge, but only that our analysis does not cover them. Second, the topologies for which the convergence is claimed in (2.13) is suboptimal when compared to the results we prove in Section 4. However, we choose to keep the statement as simple as possible. The interested reader can refer to Section 4 to get finer results, including the convergence of approximate gradients to be defined later on.

Section 5 is then devoted to the comparison of the numerical results produced by the different schemes.

3. NUMERICAL ANALYSIS FOR FIXED MESHES

In this section, one aims to show that each scheme admits at least one solution and that the physical bounds are preserved by the schemes. Our approach is based on a topological degree argument [38, 17] to be detailed in Section 3.3. It relies on a priori estimates to be stated in Section 3.2. But let us start by some preliminary properties of the different functions \mathcal{F} , defined either by (2.8), (2.9), (2.10), or (2.11), and some consequences for the inner numerical fluxes $F_{K\sigma}^n$.

3.1. Face concentration and face dissipation. For each scheme, one can naturally define a face concentration functional $\mathcal{C} : (0, 1) \times (0, 1) \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ by

$$\mathcal{C} : (c_K, c_L, \Phi_K, \Phi_L) \mapsto \frac{\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L)}{h(c_K) + \Phi_K - h(c_L) - \Phi_L}. \quad (3.1)$$

It clearly satisfies $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = \mathcal{C}(c_L, c_K, \Phi_L, \Phi_K)$. It means that we can define one unique face concentration by internal face and by choice of flux

$$\mathcal{C}_\sigma^n = \mathcal{C}(c_K^n, c_L^n, \Phi_K^n, \Phi_L^n) \quad \forall \sigma \in \mathcal{E}_{\text{int}}, \sigma = K|L \quad (3.2)$$

and that each flux $F_{K\sigma}^n$ can be rewritten as

$$F_{K\sigma}^n = -\tau_\sigma \mathcal{C}_\sigma^n D_{K\sigma}(h(\mathbf{c}^n) + \Phi^n), \quad \forall K \in \mathcal{T}, \forall \sigma = K|L. \quad (3.3)$$

We also introduce a face dissipation functional $\mathcal{D} : (0, 1) \times (0, 1) \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$, defined by

$$\mathcal{D}(c_K, c_L, \Phi_K, \Phi_L) = \mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) |h(c_K) - h(c_L) + \Phi_K - \Phi_L|^2. \quad (3.4)$$

and we set, for each scheme,

$$\mathcal{D}_\sigma^n = \mathcal{D}(c_K^n, c_L^n, \Phi_K^n, \Phi_L^n), \quad \forall \sigma \in \mathcal{E}_{\text{int}}, \sigma = K|L. \quad (3.5) \quad \{\text{eq:Dsig}\}$$

For $\delta \in (0, 1)$ and $M \in \mathbb{R}$, we finally define two functions associated to \mathcal{D} , $\Psi_{\delta, M} : (0, 1) \rightarrow \mathbb{R}$ and $\Upsilon_{\delta, M} : (0, 1) \rightarrow \mathbb{R}$, by

$$\begin{aligned} \Psi_{\delta, M}(c_L) &= \inf\{\mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in [\delta, 1), (\Phi_K, \Phi_L) \in [-M, M]^2\} \\ \Upsilon_{\delta, M}(c_L) &= \inf\{\mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in (0, 1 - \delta], (\Phi_K, \Phi_L) \in [-M, M]^2\} \end{aligned} \quad (3.6) \quad \{\text{eq:defPsi}\}$$

Note that $\delta \mapsto \Psi_{\delta, M}(c_L)$ and $\delta \mapsto \Upsilon_{\delta, M}(c_L)$ are nondecreasing for all $M \in \mathbb{R}$ and all $c_L \in (0, 1)$.

Our first lemma in this section focuses on the face concentration, which for three scheme over four can be shown to be an average value of the surrounding cell concentrations.

lem: avg

Lemma 3.1. *The face concentration functional defined by (3.1) and either (2.8), (2.9) or (2.11) verifies, for all $(c_K, c_L, \Phi_K, \Phi_L) \in (0, 1) \times (0, 1) \times \mathbb{R} \times \mathbb{R}$,*

$$\min(c_K, c_L) \leq \mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) \leq \max(c_K, c_L). \quad (3.7) \quad \{\text{eq:avg}\}$$

Property (3.7) does not hold in general in the case where \mathcal{F} is defined by (2.10) (activity based flux), but one still has, for all $(c_K, c_L, \Phi_K, \Phi_L) \in (0, 1) \times (0, 1) \times \mathbb{R} \times \mathbb{R}$,

$$\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) \geq \frac{\min(c_K, c_L)}{2} > 0. \quad (3.8) \quad \{\text{eq:avgA}\}$$

Proof. We first remark that Property (3.7) trivially holds for the centered flux (2.8) since, in this case,

$$\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = \frac{c_K + c_L}{2}.$$

The proof is more intricate for the Sedan flux (2.9) and the Bessemoulin-Chatard flux (2.11). It relies on elementary properties of the Bernoulli function.

Let us start with the Bessemoulin-Chatard flux (2.11), for which

$$\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = \frac{dr_\sigma \left(B \left(\frac{\Phi_L - \Phi_K}{dr_\sigma} \right) c_K - B \left(\frac{\Phi_K - \Phi_L}{dr_\sigma} \right) c_L \right)}{h(c_K) + \Phi_K - h(c_L) - \Phi_L}, \quad (3.9) \quad \{\text{eq:bchD}\}$$

where we have set

$$dr_\sigma = dr(c_K, c_L). \quad (3.10) \quad \{\text{eq:dr_sig}\}$$

Let us now recall the elementary property of the Bernoulli function:

$$B(\log(a) - \log(b))a - B(\log(b) - \log(a))b = 0, \quad \forall (a, b) \in (0, 1)^2. \quad (3.11) \quad \{\text{eq:logBer}\}$$

Introducing the quantities $x = \log(c_K/c_L)$ and $y = (\Phi_L - \Phi_K)/dr_\sigma$, elementary calculations show that the relation (3.9) rewrites

$$\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = \frac{B(y) - B(x)}{x - y} c_K + \frac{B(-x) - B(-y)}{x - y} c_L. \quad (3.12) \quad \{\text{eq:B_avg}\}$$

But, the Bernoulli function is decreasing and satisfies $B(x) - B(-x) = -x$ for all $x \in \mathbb{R}$, which implies

$$\frac{B(y) - B(x)}{x - y} + \frac{B(-x) - B(-y)}{x - y} = 1.$$

Thus $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L)$ is a convex combination of c_K and c_L , so that (3.7) holds for the Bessemoulin-Chatard flux.

The case of the Sedan flux (2.9) can be treated similarly because (3.12) is still satisfied, but with $x = \log(c_K/c_L)$ and $y = \Phi_L + \nu(c_L) - \Phi_K + \nu(c_K)$. Here again, $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L)$ is a convex combination of c_K and c_L , so that (3.7) holds for the Sedan flux.

The fact that (3.7) does not hold for the activity based flux (2.10) is depicted on Figure 2. Nevertheless, one can express the corresponding face concentration under the form

$$\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = \frac{\beta(c_K) + \beta(c_L)}{2} \times \left(\frac{B(y) - B(x)}{x - y} a(c_K) + \frac{B(-x) - B(-y)}{x - y} a(c_L) \right),$$

with $x = \log(a(c_K)) - \log(a(c_L))$ and $y = \Phi_L - \Phi_K$. Therefore, $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L)$ is the product of the arithmetic mean of the positive quantities $\beta(c_K)$ and $\beta(c_L)$ with a convex combination of the positive quantities $a(c_K)$ and $a(c_L)$. As a is increasing, this convex combination is bounded by below by $a(\min(c_K, c_L))$. Using the identity $\beta(c)a(c) = c$, we get (3.8). \square

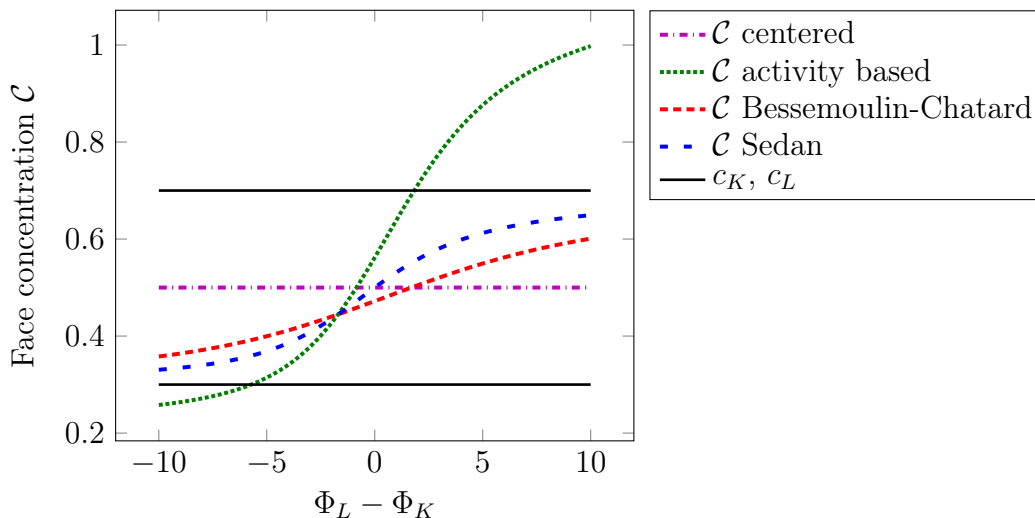


FIGURE 2. Evolution of the face concentration $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L)$ as a function of the jump of the potential $\Phi_L - \Phi_K$ for the choice $c_K = 0.3$ and $c_L = 0.7$.

fig:EC

As a by-product of Lemma 3.1, we obtain that the face dissipation \mathcal{D} is a nonnegative function as the product of nonnegative quantities. The second lemma of this section is about the coercivity of the face dissipation functional. As its proof is technical, it is given in Appendix B.

Lemma 3.2. *The face dissipation functional defined by (3.4) and either (2.8), (2.9), (2.10) or (2.11) satisfies the following dissipation property: given $\delta \in (0, 1)$ and $M \in \mathbb{R}$, there holds, for Ψ and Υ as defined in (3.6):*

$$\begin{aligned} \lim_{c_L \rightarrow 0} \Psi_{\delta, M}(c_L) &= +\infty, \\ \lim_{c_L \rightarrow 1} \Upsilon_{\delta, M}(c_L) &= +\infty. \end{aligned}$$

3.2. Uniform a priori estimates. In all this section, we assume that $(\mathbf{c}^n, \Phi^n)_{1 \leq n \leq N}$ is a solution to the scheme (2.3)–(2.6) with a numerical flux defined among (2.8)–(2.11). We also assume that this solution verifies: $0 < c_K^n < 1$ for all $K \in \mathcal{T}$ and all $1 \leq n \leq N$. Then the goal of this section is to derive enough a priori estimates on $(\mathbf{c}^n, \Phi^n)_{1 \leq n \leq N}$ in order to show the existence of a weak solution to the nonlinear system induced by the scheme.

The first lemma is the discrete counterpart of the global conservation of mass.

lem:dissip

ec:apriori

lem:mass

Lemma 3.3. *One has*

$$\sum_{K \in \mathcal{T}} m_K c_K^n = \sum_{K \in \mathcal{T}} m_K c_K^{n-1} = \int_{\Omega} c^0 d\mathbf{x}, \quad \forall 1 \leq n \leq N.$$

Proof. The first equality is obtained by summing (2.4b) over $K \in \mathcal{T}$ and by using the no-flux boundary conditions (2.5) and the local conservativity of the scheme (2.7). A straightforward induction ensures the second equality thanks to (2.1). \square

The second a priori estimate is related to energy dissipation and can be seen as a discrete counterpart of Proposition 1.1.

prop:E_disc

Proposition 3.1. *There holds*

$$\frac{E_{\mathcal{T}}(\mathbf{c}^n, \Phi^n) - E_{\mathcal{T}}(\mathbf{c}^{n-1}, \Phi^{n-1})}{\Delta t_n} \leq - \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} \mathcal{D}_{\sigma}^n \leq 0, \quad \forall 1 \leq n \leq N,$$

with \mathcal{D}_{σ}^n defined by (3.5), and $E_{\mathcal{T}}$ defined by (2.12).

Proof. Due to the convexity of H and of $x \mapsto x^2/2$, we have :

$$\begin{aligned} E_{\mathcal{T}}(\mathbf{c}^n, \Phi^n) - E_{\mathcal{T}}(\mathbf{c}^{n-1}, \Phi^{n-1}) &\leq \sum_{K \in \mathcal{T}} m_K (c_K^n - c_K^{n-1}) h(c_K^n) + \\ &\sum_{\sigma \in \mathcal{E}} \tau_{\sigma} D_{\sigma} \Phi^n D_{\sigma} (\Phi^n - \Phi^{n-1}) - \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}^D \cap \mathcal{E}_K} \tau_{\sigma} \Phi_{\sigma}^D D_{K\sigma} (\Phi^n - \Phi^{n-1}). \end{aligned}$$

A discrete integration by parts permits to rewrite the sum of the two last terms, which, combined to the scheme (2.4a), leads to

$$E_{\mathcal{T}}(\mathbf{c}^n, \Phi^n) - E_{\mathcal{T}}(\mathbf{c}^{n-1}, \Phi^{n-1}) \leq \sum_{K \in \mathcal{T}} m_K (c_K^n - c_K^{n-1}) (h(c_K^n) + \Phi_K^n). \quad (3.13) \quad \{\text{E:step1}\}$$

Multiplying the equation (2.4b) by $h(c_K^n) + \Phi_K^n$ and summing over $K \in \mathcal{T}$, we obtain that

$$\begin{aligned} \sum_{K \in \mathcal{T}} m_K \frac{c_K^n - c_K^{n-1}}{\Delta t_n} (h(c_K^n) + \Phi_K^n) &= - \sum_{K \in \mathcal{T}} (h(c_K^n) + \Phi_K^n) \sum_{\sigma \in \mathcal{E}_K} F_{K\sigma}^n \\ &= - \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} \mathcal{C}_{\sigma}^n |D_{\sigma} (h(\mathbf{c}^n) + \Phi^n)|^2 \quad (3.14) \quad \{\text{E:step2}\} \end{aligned}$$

Combining (3.13) and (3.14) provides the desired estimate. \square

The third statement of this section is devoted to a uniform L^{∞} estimate of $(\Phi^n)_{1 \leq n \leq N}$. It is a straightforward consequence of the slightly more general Proposition A.1 stated in appendix, together with the a priori bounds $0 < c_K^n < 1$ and $-\|c^{dp}\|_{\infty} \leq c_K^{dp} \leq \|c^{dp}\|_{\infty}$.

em:LinPhi

Lemma 3.4. *There exists M_{Φ} depending only on Φ^D , c^{dp} and Ω such that*

$$|\Phi_K^n| \leq M_{\Phi}, \quad \forall K \in \mathcal{T}, \forall 1 \leq n \leq N.$$

Next lemma concerns the discrete $L^{\infty}((0, T); H^1(\Omega))$ estimate on the electric potential.

:LinH1Phi

Lemma 3.5. *There exists C depending only on Φ^D , c^{dp} , Ω and $\zeta_{\mathcal{T}}$ such that*

$$\begin{aligned} \sum_{\sigma \in \mathcal{E}} \tau_{\sigma} |D_{\sigma} \Phi^n|^2 &\leq C, \quad \forall 1 \leq n \leq N \\ \text{and } \left| \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}^D \cap \mathcal{E}_K} \tau_{\sigma} \Phi_{\sigma}^D D_{K\sigma} \Phi^n \right| &\leq C, \quad \forall 1 \leq n \leq N. \end{aligned}$$

Proof. As $\Phi^D \in L^\infty \cap H^1(\Omega)$, it is discretized into $\Phi^D \in \mathbb{R}^{\mathcal{T}}$ by setting

$$\Phi_K^D = \frac{1}{m_K} \int_K \Phi^D d\mathbf{x}, \quad \forall K \in \mathcal{T}, \quad \text{and} \quad \Phi_\sigma^D = \frac{1}{m_\sigma} \int_\sigma \Phi^D d\gamma, \quad \forall \sigma \in \mathcal{E}^D.$$

It satisfies $|\Phi_K^D| \leq \|\Phi^D\|_\infty$ for all $K \in \mathcal{T}$. Multiplying (2.4a) by $\Phi_K^n - \Phi_K^D$ and summing over $K \in \mathcal{T}$ provides

$$\sum_{\sigma \in \mathcal{E}} \tau_\sigma D_{K\sigma} \Phi^n D_{K\sigma} (\Phi^n - \Phi^D) = \sum_{K \in \mathcal{T}} m_K (c_K^n + c_K^{dp}) (\Phi_K^n - \Phi_K^D). \quad (3.15) \quad \{\text{eq:AB}\}$$

Using the elementary inequality $a(a-b) \geq \frac{a^2-b^2}{2}$, we get that

$$\sum_{\sigma \in \mathcal{E}} \tau_\sigma D_{K\sigma} \Phi^n D_{K\sigma} (\Phi^n - \Phi^D) \geq \frac{1}{2} \sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma \Phi^n)^2 - \frac{1}{2} \sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma \Phi^D)^2.$$

Using the boundedness of c_K^n , c_K^{dp} , Φ_K^D , and of Φ_K^n (cf. Lemma 3.4), we obtain that the right-hand side is bounded:

$$\sum_{K \in \mathcal{T}} m_K (c_K^n + c_K^{dp}) (\Phi_K^n - \Phi_K^D) \leq C.$$

Following [25, Lemma 13.4], there exists C depending only on $\zeta_{\mathcal{T}}$ such that

$$\sum_{\sigma \in \mathcal{E}} \tau_\sigma (D_\sigma \Phi^D)^2 \leq C \|\Phi^D\|_{H^1(\Omega)}^2, \quad (3.16) \quad \{\text{eq:H1PhiD}\}$$

which allows to conclude the proof of the first inequality of Lemma 3.5. Multiplying now the scheme (2.4a) by Φ_K^n and summing over $K \in \mathcal{T}$ leads to the second inequality by following the same kind of computations. \square

Remark 3.1. Using Proposition 3.1, we notice that Lemma 3.5 implies the existence of C depending only on c^0 , Φ^D , Ω and $\zeta_{\mathcal{T}}$ such that:

$$\sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma \mathcal{D}_\sigma^n \leq C, \quad \forall N \in \mathbb{N}$$

As a last step before establishing the existence of a solution to the scheme, we show that the approximate concentrations c^n are bounded away from 0 and 1. Note that contrary to Lemmas 3.3 and 3.4 and to Proposition 3.1, the estimate of the following Lemma is not uniform with respect to mesh size and time step.

Lemma 3.6. *There exists $\epsilon > 0$ depending on \mathcal{T} , Δt , Φ^D , \bar{c} , c^{dp} and Ω such that*

$$\epsilon < c_K^n < 1 - \epsilon, \quad \forall K \in \mathcal{T}, \quad \forall 1 \leq n \leq N.$$

Proof. The proof follows the idea of [11, Lemma 3.10] (see also [12, Lemma 3.7]). Let us establish the lower bound, since the outline of the proof of the upper bound is similar. Here again, we drop the superscript j for the ease of reading.

Because of assumption (1.4) on the initial data and of the choice (2.1) for its discretization, one knows that

$$\frac{1}{m_\Omega} \sum_{K \in \mathcal{T}} m_K c_K^0 = \bar{c} \in (0, 1).$$

Lemma 3.3 ensures the conservation of mass, so that

$$\frac{1}{m_\Omega} \sum_{K \in \mathcal{T}} m_K c_K^n = \bar{c} \in (0, 1), \quad \forall n \geq 1.$$

This implies that there exists $K_0 \in \mathcal{T}$ such that $c_{K_0}^n \geq \bar{c} > 0$. We set $\delta_0 = \bar{c}$.

rem:D_T2

em:epsilon

Denote by $\Phi[\mathbf{c}^n]$ the unique solution to the linear system (2.4a). Lemma 3.5 ensures that the functional $\mathbf{c}^n \mapsto E_{\mathcal{T}}(\mathbf{c}^n, \Phi[\mathbf{c}^n])$ is bounded on $(0, 1)^{\mathcal{T}}$. Therefore, it follows from Proposition 3.1 that there exists $C_{\mathcal{D}}$ depending (among others) on Δt_n such that

$$\mathcal{D}_{\mathcal{T}}^n = \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} \mathcal{D}_{\sigma}^n \leq C_{\mathcal{D}}, \quad \forall 1 \leq n \leq N. \quad (3.17) \quad \{\text{eq:D_T2}\}$$

In particular, for all face $\sigma \in \mathcal{E}_{K_0}$, one gets that $\tau_{\sigma} \mathcal{D}_{\sigma}^n \leq C_{\mathcal{D}}$. Therefore, the concentration $c_{K_1}^n$ in any neighboring cell K_1 of K_0 is bounded away from 0 by

$$\begin{aligned} c_{K_1}^n &\geq \inf \left\{ c_L \in (0, 1) ; \Psi_{c_{K_0}^n, M_{\Phi}}(c_L) \leq C_{\mathcal{D}}/\tau_{\sigma} \right\} \\ &\geq \inf \left\{ c_L \in (0, 1) ; \Psi_{\delta_0, M_{\Phi}}(c_L) \leq C_{\mathcal{D}}/\min_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} \right\} =: \delta_1 > 0 \end{aligned}$$

thanks to the monotonicity of $\delta \mapsto \Psi_{\delta, M}(c_L)$. Owing to Lemma 3.2, the above right-hand side is bounded away from 0 by some quantity that might also depends on \mathcal{T} because of the presence of τ_{σ} . This lower bound can be set to δ_1 and we can then iterate the procedure to the neighboring cells of K_1 , and so on and so forth. Since the mesh is finite, only a finite number of iterations $I_{\mathcal{T}}$ is needed to cover all the cells, whence a uniform lower bound on c_K^n : $\epsilon = \min_{1 \leq i \leq I_{\mathcal{T}}} \delta_i$, where

$$\delta_{i+1} = \inf \left\{ c_L \in (0, 1) ; \Psi_{\delta_i, M_{\Phi}}(c_L) \leq C_{\mathcal{D}}/\min_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} \right\} > 0, \quad \delta_0 = \bar{c}.$$

□

:existence

3.3. Existence of a solution to the schemes. Based on the estimates derived in the previous section, we can establish the existence of at least one solution to each scheme. This completes the proof of Theorem 2.1.

:existence

Proposition 3.2. *Let \mathbf{c}^0 be defined by (2.1). Then, for all $1 \leq n \leq N$, the nonlinear system of equations (2.3)–(2.6), supplemented either with (2.8), (2.9), (2.10), or (2.11), has a solution $(\mathbf{c}^n, \Phi^n) \in \mathbb{R}^{\mathcal{T}} \times \mathbb{R}^{\mathcal{T}}$.*

Proof. The proof is a proof by induction; it relies on a topological degree argument [38, 17] at each time step. The idea is to transform in a continuous way our complex nonlinear system into a linear system while guaranteeing that a priori estimates controlling the solution remain valid all along the homotopy. We sketch the main ideas of the proof, making the homotopy (parametrized by $\lambda \in [0, 3]$) explicit.

We denote by $\mathbf{c}^* = \mathbf{c}^{n-1} \in (0, 1)^{\mathcal{T}}$ the discrete concentration at the previous time step. We are interested in the existence of zeros for a functional

$$\mathcal{H} : \begin{cases} [0, 3] \times (0, 1)^{\mathcal{T}} \times \mathbb{R}^{\mathcal{T}} \rightarrow \mathbb{R}^{\mathcal{T}} \times \mathbb{R}^{\mathcal{T}} \\ (\lambda, \mathbf{c}, \Phi) \mapsto \mathcal{H}(\lambda, \mathbf{c}, \Phi) \end{cases}$$

that boils down to the scheme (2.4) when $\lambda = 3$. For sake of simplicity, instead of giving the definition of \mathcal{H} for the different values of λ , we give a sense to the fact that $\mathbf{c}^{(\lambda)}, \Phi^{(\lambda)}$ is solution to $\mathcal{H}(\lambda, \mathbf{c}^{(\lambda)}, \Phi^{(\lambda)}) = 0$.

We start with $\lambda \in [0, 1]$: $\mathbf{c}^{(\lambda)}$ is defined as the solution to the nonlinear system of equation

$$m_K \frac{c_K^{(\lambda)} - c_K^*}{\Delta t_n} + (1 - \lambda) \sum_{\sigma \in \mathcal{E}_{K, \text{int}}} \tau_{\sigma} (c_K^{(\lambda)} - c_L^{(\lambda)}) + \lambda \sum_{\sigma \in \mathcal{E}_{K, \text{int}}} \tau_{\sigma} \left(r(c_K^{(\lambda)}) - r(c_L^{(\lambda)}) \right) = 0, \quad (3.18) \quad \{\text{eq:lambda}\}$$

while $\Phi^{(\lambda)} = 0$. Let us remark that for $\lambda = 0$, it boils down to an invertible linear system of equations. Moreover, adapting the proof of Proposition 3.1 and using the property $(r(a) - r(b))(h(a) - h(b)) \geq (a - b)(h(a) - h(b))$ for all $(a, b) \in (0, 1)^2$, we get:

$$E_{\mathcal{T}}(\mathbf{c}^{(\lambda)}, \mathbf{0}) - E_{\mathcal{T}}(\mathbf{c}^*, \mathbf{0}) \leq -\Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} (c_K^{(\lambda)} - c_L^{(\lambda)}) (h(c_K^{(\lambda)}) - h(c_L^{(\lambda)})).$$

As the associated dissipation function defined by $\mathcal{D}(c_K, c_L) = (c_K - c_L)(h(c_K) - h(c_L))$ is clearly coercive in the sense of Lemma 3.2, we can deduce as in Lemma 3.6 the existence of $\epsilon_1 > 0$ such that $\epsilon_1 < c_K^{(\lambda)} < 1 - \epsilon_1$ for all $K \in \mathcal{T}$ and for all $\lambda \in [0, 1]$.

For $\lambda \in [1, 2]$, one lets our system evolve from the monotone scheme corresponding to $\lambda = 1$ (which, due to Remark 2.1 corresponds to the Sedan scheme for the case without electrical potential) to the scheme with the expected numerical fluxes $F_{K\sigma}$. But the electrical potential is still blocked to $\Phi^{(\lambda)} = \mathbf{0}$, i.e.,

$$m_K \frac{c_K^{(\lambda)} - c_K^*}{\Delta t_n} + (2 - \lambda) \sum_{\sigma \in \mathcal{E}_{K,\text{int}}} \tau_{\sigma} \left(r(c_K^{(\lambda)}) - r(c_L^{(\lambda)}) \right) + (\lambda - 1) \sum_{\sigma \in \mathcal{E}_{K,\text{int}}} F_{K\sigma}^{(\lambda)} = 0, \quad (3.19)$$

$$F_{K\sigma}^{(\lambda)} = \tau_{\sigma} \mathcal{F}(c_K^{(\lambda)}, c_L^{(\lambda)}, 0, 0).$$

{eq: lambda

with \mathcal{F} defined either by (2.8), (2.9), (2.10), or (2.11). Thanks to Lemma 3.6, there exists $\epsilon_2 > 0$ such that $\epsilon_2 < c_K^{(\lambda)} < 1 - \epsilon_2$ for all $K \in \mathcal{T}$ and for all $\lambda \in [1, 2]$.

During the last step, $\lambda \in [2, 3]$, we reactivate progressively the electrical potential while keeping equation (2.4b). Defining

$$\Phi_{\sigma}^{D,(\lambda)} = (\lambda - 2)\Phi_{\sigma}^D, \quad \forall \sigma \in \mathcal{E}^D,$$

$(\mathbf{c}^{(\lambda)}, \Phi^{(\lambda)})$ is defined, for all $\lambda \in [2, 3]$ as the solution to the nonlinear system: for all $K \in \mathcal{T}$,

$$m_K \frac{c_K^{(\lambda)} - c_K^*}{\Delta t_n} + \sum_{\sigma \in \mathcal{E}_{K,\text{int}}} F_{K\sigma}^{(\lambda)} = 0, \quad \text{with } F_{K\sigma}^{(\lambda)} = \tau_{\sigma} \mathcal{F}(c_K^{(\lambda)}, c_L^{(\lambda)}, (\lambda - 2)\Phi_K^{(\lambda)}, (\lambda - 2)\Phi_L^{(\lambda)}),$$

$$- \sum_{\sigma \in \mathcal{E}_K} \tau_{\sigma} D_{K\sigma} \Phi^{(\lambda)} = (\lambda - 2)m_K (c_K^{(\lambda)} + c_K^{dp}).$$

Thanks to Proposition A.1, one has $|\Phi_K^{(\lambda)}| \leq M_{\Phi}$ for all $K \in \mathcal{T}$ and for all $\lambda \in [2, 3]$.

Moreover, as in Lemma 3.6, we can establish the existence of $\epsilon_3 > 0$ such that $\epsilon_3 < c_K^{(\lambda)} < 1 - \epsilon_3$ for all $K \in \mathcal{T}$ and for all $\lambda \in [2, 3]$.

Finally, all along the homotopy parametrized by $\lambda \in [0, 3]$, the solution $(\mathbf{c}^{(\lambda)}, \Phi^{(\lambda)})$ remains inside the compact subset $[\epsilon, 1 - \epsilon]^{\mathcal{T}} \times [-M_{\Phi} - 1, M_{\Phi} + 1]^{\mathcal{T}}$ with $\epsilon = \min(\epsilon_1, \epsilon_2, \epsilon_3)$. Thus the topological degree corresponding to $\mathcal{H}(\lambda, \mathbf{c}, \Phi) = \mathbf{0}$ and to the set $[\epsilon, 1 - \epsilon]^{\mathcal{T}} \times [-M_{\Phi} - 1, M_{\Phi} + 1]^{\mathcal{T}}$ is equal to one all along the homotopy and in particular for $\lambda = 3$. This ensures the existence of (at least) one solution to the scheme (2.4). \square

4. ABOUT THE CONVERGENCE TOWARDS A WEAK SOLUTION

The goal of this section is to prove Theorem 2.2, which states the convergence of the centered scheme (2.4), (2.8), and the Sedan scheme (2.4), (2.9), towards a weak solution to the continuous problem in the sense of Definition 1. Unfortunately, the proof we propose here neither applies to the activity base scheme (2.4), (2.10), nor to the Bessemoulin-Chatard scheme (2.4), (2.11). This does not mean that these schemes do not converge. Indeed, numerical evidences provided in Section 5 seem to show that all the four schemes converge.

onvergence

We consider here a sequence $(\mathcal{T}_m, \mathcal{E}_m, (\mathbf{x}_K)_{K \in \mathcal{T}_m})_{m \geq 1}$ of admissible discretization with $h_{\mathcal{T}_m}, \overline{\Delta t}_m$ tending to 0 as m tends to $+\infty$, while the regularity $\zeta_{\mathcal{T}_m}$ remains uniformly bounded from below by a positive constant ζ^* . Theorem 2.1 provides the existence of a family of discrete solutions $(\mathbf{c}_m, \Phi_m)_m = \left((c_K^n)_{K \in \mathcal{T}_m, 1 \leq n \leq N_m}, (\Phi_K^n)_{K \in \mathcal{T}_m, 1 \leq n \leq N_m} \right)$. To prove Theorem 2.2, we first establish in Section 4.2 some compactness properties on the family of piecewise constant approximate solutions $(c_{\mathcal{T}_m, \Delta t_m}, \Phi_{\mathcal{T}_m, \Delta t_m})$ satisfied by the centered scheme and the Sedan scheme. Then we identify the limit as a weak solution in Section 4.3.

In order to enlighten the notations, we remove the subscript m as soon as it is not necessary for understanding.

reconstruct

4.1. Reconstruction operators. In order to carry out the analysis of convergence, we introduce some reconstruction operators following the methodology proposed in [22].

The operators $\pi_{\mathcal{T}} : \mathbb{R}^{\mathcal{T}} \rightarrow L^\infty(\Omega)$ and $\pi_{\mathcal{T}, \Delta t} : \mathbb{R}^{\mathcal{T} \times N} \rightarrow L^\infty((0, T) \times \Omega)$ are defined respectively by

$$\pi_{\mathcal{T}} \mathbf{u}(\mathbf{x}) = u_K \quad \text{if } \mathbf{x} \in K, \quad \forall \mathbf{u} = (u_K)_{K \in \mathcal{T}},$$

and

$$\pi_{\mathcal{T}, \Delta t} \mathbf{u}(t, \mathbf{x}) = u_K^n \quad \text{if } (t, \mathbf{x}) \in (t_{n-1}, t_n] \times K, \quad \forall \mathbf{u} = (u_K^n)_{K \in \mathcal{T}, 1 \leq n \leq N}.$$

These operators allow to pass from the discrete solution $(\mathbf{c}^n, \Phi^n)_{1 \leq n \leq N}$ to the approximate solution since

$$c_{\mathcal{T}, \Delta t} = \pi_{\mathcal{T}, \Delta t} (\mathbf{c}^n)_n, \quad \Phi_{\mathcal{T}, \Delta t} = \pi_{\mathcal{T}, \Delta t} (\Phi^n)_n.$$

But in order to carry out the analysis, we further need to introduce approximate gradient reconstruction. Since the boundary conditions play a crucial role in the definition of the gradient, we need to enrich the discrete solution by face values $(c_\sigma^n)_{\sigma \in \mathcal{E}_{\text{ext}}, 1 \leq n \leq N}$ and $(\Phi_\sigma^n)_{\sigma \in \mathcal{E}_{\text{ext}}, 1 \leq n \leq N}$ defined by $c_\sigma^n = c_{K\sigma}^n$ and $\Phi_\sigma^n = \Phi_{K\sigma}^n$. With a slight abuse of notations, we still denote by $\mathbf{c}^n = ((c_K^n)_{K \in \mathcal{T}}, (c_\sigma^n)_{\sigma \in \mathcal{E}_{\text{ext}}})$ and $\Phi^n = ((\Phi_K^n)_{K \in \mathcal{T}}, (\Phi_\sigma^n)_{\sigma \in \mathcal{E}_{\text{ext}}})$ the elements of $(0, 1)^{\mathcal{T} + \mathcal{E}_{\text{ext}}}$ and $\mathbb{R}^{\mathcal{T} + \mathcal{E}_{\text{ext}}}$ containing both the cell values and the exterior faces values of the concentration and the potential respectively.

For $\sigma = K|L \in \mathcal{E}_{\text{int}}$, we denote by Δ_σ the diamond cell corresponding to σ , that is the interior of the convex hull of $\{\sigma, \mathbf{x}_K, \mathbf{x}_L\}$. For $\sigma \in \mathcal{E}_{\text{ext}}$, the diamond cell Δ_σ is defined as the interior of the convex hull of $\{\sigma, \mathbf{x}_K\}$. The approximate gradient $\nabla_{\mathcal{T}} : \mathbb{R}^{\mathcal{T} + \mathcal{E}_{\text{ext}}} \rightarrow L^2(\Omega)^d$ we use in the analysis is merely weakly consistent (unless $d = 1$) and takes its source in [14, 23]. It is piecewise constant on the diamond cells Δ_σ , and it is defined as follows:

$$\nabla_{\mathcal{T}} \mathbf{u}(\mathbf{x}) = -d \frac{D_{K\sigma} \mathbf{u}}{d_\sigma} \mathbf{n}_{K\sigma} \quad \text{if } \mathbf{x} \in \Delta_\sigma, \quad \forall \mathbf{u} \in \mathbb{R}^{\mathcal{T} + \mathcal{E}_{\text{ext}}}.$$

We also define $\nabla_{\mathcal{T}, \Delta t} : \mathbb{R}^{(\mathcal{T} + \mathcal{E}_{\text{ext}}) \times N} \rightarrow L^2(Q_T)^d$ by setting

$$\nabla_{\mathcal{T}, \Delta t} \mathbf{u}(t, \cdot) = \nabla_{\mathcal{T}} \mathbf{u}^n \quad \text{if } t \in (t_{n-1}, t_n], \quad \forall \mathbf{u} = (\mathbf{u}^n)_{1 \leq n \leq N} \in \mathbb{R}^{(\mathcal{T} + \mathcal{E}_{\text{ext}}) \times N}.$$

Let us recall now some key properties to be used in the analysis. First, for all $\mathbf{u}, \mathbf{v} \in \mathbb{R}^{\mathcal{T} + \mathcal{E}_{\text{ext}}}$, there holds

$$\sum_{\sigma \in \mathcal{E}} \tau_\sigma D_{K\sigma} \mathbf{u} D_{K\sigma} \mathbf{v} = \frac{1}{d} \int_{\Omega} \nabla_{\mathcal{T}} \mathbf{u} \cdot \nabla_{\mathcal{T}} \mathbf{v} \, d\mathbf{x}.$$

This implies in particular that

$$\sum_{\sigma \in \mathcal{E}} \tau_\sigma |D_\sigma \mathbf{u}|^2 = \frac{1}{d} \int_{\Omega} |\nabla_{\mathcal{T}} \mathbf{u}|^2 \, d\mathbf{x}, \quad \forall \mathbf{u} \in \mathbb{R}^{\mathcal{T} + \mathcal{E}_{\text{ext}}}. \quad (4.1)$$

{eq:norm_L

ec:compact

4.2. **Compactness properties for the approximate concentration.** The goal here is to take advantage of the a priori estimates established in Section 3.2 to recover enough compactness for the sequences of approximate solutions.

em:L2H1_xi

Lemma 4.1. *Let (\mathbf{c}_m, Φ_m) be the family of discrete solutions defined either by the centered scheme or by the Sedan scheme. There exists C depending only on Φ^D , Ω , ζ^* , c_0 , c^{dp} and T , such that*

$$\iint_{Q_T} |\nabla_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c}_m)|^2 + (\pi_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c}_m))^2 d\mathbf{x}dt \leq C.$$

Proof. We get rid of the subscript m for the ease of reading. We will split the proof in two parts, first we focus on the proof of:

$$\iint_{Q_T} |\nabla_{\mathcal{T}, \Delta t} r(\mathbf{c})|^2 d\mathbf{x}dt \leq C. \quad (4.2) \quad \{\text{eq:normL2}\}$$

Thanks to (4.1), we have

$$\begin{aligned} \iint_{Q_T} |\nabla_{\mathcal{T}, \Delta t} r(\mathbf{c})|^2 &= d \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma |D_\sigma(r(\mathbf{c}^n))|^2, \\ &= d \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma \left(\tilde{\mathcal{C}}_\sigma^n \right)^2 |D_\sigma(h(\mathbf{c}^n))|^2, \end{aligned}$$

where we have defined the mean face concentrations $\left(\tilde{\mathcal{C}}_\sigma^n \right)_{\sigma \in \mathcal{E}_{\text{int}}, 1 \leq n \leq N}$ by setting

$$\tilde{\mathcal{C}}_\sigma^n = \frac{D_\sigma r(\mathbf{c}^n)}{D_\sigma h(\mathbf{c}^n)} \text{ if } c_K^n \neq c_L^n \quad \text{and} \quad \tilde{\mathcal{C}}_\sigma^n = c_K^n \text{ otherwise,} \quad \forall \sigma = K|L. \quad (4.3) \quad \{\text{eq:wtCsig}\}$$

As noticed in Appendix C, $\tilde{\mathcal{C}}_\sigma^n$ is a mean value of c_K^n and c_L^n ; so that $\tilde{\mathcal{C}}_\sigma^n \in (0, 1)$ for all $\sigma \in \mathcal{E}_{\text{int}}$. Moreover Lemma C.1 proved in Appendix C ensures that there exists $G > 0$ such that

$$\frac{\tilde{\mathcal{C}}_\sigma^n}{\mathcal{C}_\sigma^n} \leq G, \quad \forall \sigma \in \mathcal{E}_{\text{int}}, \forall n \in \{1, \dots, N\}. \quad (4.4) \quad \{\text{eq:alacn}\}$$

Then, thanks to Young inequality, we obtain

$$\begin{aligned} \iint_{Q_T} |\nabla_{\mathcal{T}, \Delta t} r(\mathbf{c})|^2 &\leq 2dG \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma \mathcal{C}_\sigma^n |D_\sigma(h(\mathbf{c}^n) + \Phi^n)|^2 \\ &\quad + 2d \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma |D_\sigma \Phi^n|^2. \end{aligned}$$

Therefore, Remark 3.1 and Lemma 3.5 yield the desired bound (4.2).

We now focus on the proof of:

$$\iint_{Q_T} (\pi_{\mathcal{T}, \Delta t} r(\mathbf{c}))^2 d\mathbf{x}dt \leq C. \quad (4.5) \quad \{\text{eq:normL2}\}$$

Noticing that for $c^* = \frac{1+\bar{c}}{2} > \bar{c}$:

$$r(c) \leq (r(c) - r(c^*))^+ + r(c^*),$$

we have, using $(a+b)^2 \leq 2(a^2 + b^2)$:

$$\iint_{Q_T} |\pi_{\mathcal{T}, \Delta t} r(\mathbf{c})|^2 d\mathbf{x}dt \leq 2 \iint_{Q_T} |(\pi_{\mathcal{T}, \Delta t} r(\mathbf{c}) - r(c^*))^+|^2 d\mathbf{x}dt + 2r(c^*)^2 m(\Omega)T. \quad (4.6) \quad \{\text{eq:decomp}\}$$

Let $t \in [0, T]$ and $u = (\pi_{\mathcal{T}, \Delta t} r(\mathbf{c}) - r(c^*))^+(t)$. We intend to show that we have a L^2 bound on u following ideas of [1, Appendix A.1]. As u is nonnegative, we have:

$$\int_{\Omega} |u - \bar{u}|^2 = \int_{u=0} \bar{u}^2 + \int_{\Omega \setminus \{u=0\}} |u - \bar{u}|^2 \geq m(\{u=0\}) \bar{u}^2, \quad (4.7) \quad \boxed{\text{feq:firstb}}$$

where $\bar{u} = \oint_{\Omega} u$. Using Poincaré-Wirtinger inequality (see [4, Theorem 5] or [34, Theorem 2.1]), we have:

$$\int_{\Omega} |u - \bar{u}|^2 \leq \frac{C}{\zeta_{\mathcal{T}}} \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} (D_{\sigma} u)^2. \quad (4.8) \quad \boxed{\text{feq:Poinca}}$$

If we had a lower bound on $m(\{u=0\})$, the equations (4.8) and (4.7) would yield an upper bound on \bar{u} . By definition of u and monotonicity of r , u is zero if and only if c is smaller than c^* . Using the monotonicity of integration and Lemma 3.3, we have:

$$c^*(m(\Omega) - m(\{u=0\})) = \int_{c > c^*} c^* \leq \int_{\Omega} \pi_{\mathcal{T}, \Delta t} \mathbf{c}(t) = m(\Omega) \bar{c}.$$

Hence, as $c^* = (1 + \bar{c})/2$,

$$m(\Omega) \frac{1 - \bar{c}}{1 + \bar{c}} \leq m(\{u=0\}).$$

Finally, we have:

$$\int_{\Omega} u^2 \leq 2 \left(\int_{\Omega} |u - \bar{u}|^2 + \bar{u}^2 \right) \leq C \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} (D_{\sigma} u)^2.$$

Using the definition of u , we have:

$$\sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_{\sigma} (D_{\sigma} u)^2 \leq \int_{\Omega} |\nabla_{\mathcal{T}, \Delta t} r(\mathbf{c})(t)|^2.$$

Hence, integrating in time, and using 4.6:

$$\iint_{Q_T} |\pi_{\mathcal{T}, \Delta t} r(\mathbf{c})|^2 dx dt \leq C \iint_{Q_T} |\nabla_{\mathcal{T}, \Delta t} r(\mathbf{c})(t)|^2 + C.$$

We then deduce (4.5) from (4.2). It concludes the proof of Lemma 4.1. \square

op:compact

Proposition 4.1. *Let (\mathbf{c}_m, Φ_m) be the family of discrete solutions defined either by the centered scheme or by the Sedan scheme. In both cases, there exists $c \in L^{\infty}(Q_T; [0, 1])$ with $r(c) \in L^2((0, T); H^1(\Omega))$ such that, up to a subsequence,*

$$\pi_{\mathcal{T}_m, \Delta t_m} \mathbf{c}_m \xrightarrow{m \rightarrow \infty} c \quad \text{a.e. in } Q_T, \quad (4.9) \quad \boxed{\text{feq:conv_a}}$$

$$\nabla_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c}_m) \xrightarrow{m \rightarrow \infty} \nabla r(c) \quad \text{weakly in } L^2(Q_T). \quad (4.10) \quad \boxed{\text{feq:conv_g}}$$

Remark 4.1. The limit c obtained in Proposition 4.1 could *a priori* depend on the chosen subsequence or be different for the centered scheme and the Sedan scheme. In Section 4.3, we will identify each limit as a weak solution to the initial problem.

Proof. Since $0 < \pi_{\mathcal{T}_m, \Delta t_m} \mathbf{c}_m < 1$ for all $m \geq 1$, there exists $c \in L^{\infty}(Q_T; [0, 1])$ such that $\pi_{\mathcal{T}_m, \Delta t_m} \mathbf{c}_m$ tends to c in the $L^{\infty}(Q_T)$ weak- \star sense. We still have to establish the almost everywhere convergence as well as the fact that $r(c)$ belongs to $L^2((0, T); H^1(\Omega))$. To this end, we make use of the blackbox [2, Theorem 3.9] which provides both the almost everywhere convergence and the identification of the limit of $\pi_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c}_m)$ as $r(c)$. We already have Lemma 4.1 at hand and c is bounded in L^{∞} , so that, owing to [2], it

is sufficient to prove that there exists some C not depending on m such that, for all $\varphi_m = (\varphi_K, \varphi_\sigma)_{K,\sigma} \in \mathbb{R}^{(\mathcal{T}_m + \mathcal{E}_{\text{ext},m}) \times \Delta t_m}$, there holds

$$\left| \sum_n \Delta t_n \sum_{K \in \mathcal{T}_m} m_K \frac{c_K^n - c_K^{n-1}}{\Delta t_n} \varphi_K^n \right| \leq C \|\nabla_{\mathcal{T}_m, \Delta t_m} \varphi_m\|_{L^\infty(Q_T)}, \quad (4.11) \quad \boxed{\text{eq:ACM17}}$$

for having, among other things, the desired convergence (4.9). Using (2.4b) and the writing (3.3) of the fluxes, we obtain that

$$\begin{aligned} \left| \sum_n \Delta t_n \sum_{K \in \mathcal{T}_m} m_K \frac{c_K^n - c_K^{n-1}}{\Delta t_n} \varphi_K^n \right| &= \left| \sum_n \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma c_\sigma^n D_{K\sigma}(h(c^n) + \Phi^n) D_{K\sigma} \varphi \right| \\ &\leq \left(\sum_n \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma c_\sigma^n |D_\sigma(h(c^n) + \Phi^n)|^2 \right)^{1/2} \\ &\quad \times \left(\sum_n \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma |D_\sigma \varphi^n|^2 \right)^{1/2} \\ &\leq C \|\nabla_{\mathcal{T}_m, \Delta t_m} \varphi_m\|_{L^2(Q_T)} \leq C \|\nabla_{\mathcal{T}_m, \Delta t_m} \varphi_m\|_{L^\infty(Q_T)}, \end{aligned}$$

thanks to the boundedness of the dissipation in Remark 3.1 which is a consequence of Proposition 3.1.

Since $\nabla_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c}_m)$ is bounded in $L^2(Q_T)^d$, it converges weakly in $L^2(Q_T)^d$ towards some \mathbf{U} . Let us show that $\mathbf{U} = \nabla r(c)$. Let $\mathbf{V} \in C_c^\infty(Q_T; \mathbb{R}^d)$ be a smooth compactly supported vector field, we set

$$\mathbf{V}_\sigma^n = \frac{1}{m_\sigma} \int_\sigma \mathbf{V}(t_n, \gamma) d\gamma, \quad \forall \sigma \in \mathcal{E}, \forall n \in \{1, \dots, N\}.$$

It permits to define a piecewise constant function on the diamond cells and the time intervals:

$$\mathbf{V}_{\mathcal{E}, \Delta t}(t, \mathbf{x}) = \mathbf{V}_\sigma^n \text{ if } (t, \mathbf{x}) \in (t_{n-1}, t_n] \times \Delta_\sigma.$$

It is clear that $\mathbf{V}_{\mathcal{E}_m, \Delta t_m}$ converges uniformly towards \mathbf{V} as $m \rightarrow \infty$ thanks to the regularity of \mathbf{V} . Then

$$\iint_{Q_T} \nabla_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c}) \cdot \mathbf{V}_{\mathcal{E}_m, \Delta t_m} d\mathbf{x} dt \xrightarrow{m \rightarrow \infty} \iint_{Q_T} \mathbf{U} \cdot \mathbf{V} d\mathbf{x} dt.$$

But, using the geometric relation $dm_{\Delta_\sigma} = d_\sigma m_\sigma$ and the definition of \mathbf{V}_σ^n , one has

$$\begin{aligned} \iint_{Q_T} \nabla_{\mathcal{T}, \Delta t} r(\mathbf{c}) \cdot \mathbf{V}_{\mathcal{E}, \Delta t} d\mathbf{x} dt &= \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} dm_{\Delta_\sigma} \frac{r(c_{K\sigma}^n) - r(c_K^n)}{d_\sigma} \mathbf{n}_{K\sigma} \cdot \mathbf{V}_\sigma^n \\ &= - \sum_{n=1}^N \Delta t_n r(c_K^n) \sum_{\sigma \in \mathcal{E}_K} \int_\sigma \mathbf{V}(\gamma, t_n) \cdot \mathbf{n}_{K\sigma} d\gamma = - \sum_{n=1}^N \Delta t_n r(c_K^n) \int_K \text{div}(\mathbf{V}(\mathbf{x}, t_n)) d\mathbf{x}. \end{aligned}$$

We deduce from the convergence of $\pi_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c})$ towards $r(c)$ that

$$\iint_{Q_T} \nabla_{\mathcal{T}_m, \Delta t_m} r(\mathbf{c}) \cdot \mathbf{V}_{\mathcal{E}_m, \Delta t_m} d\mathbf{x} dt \xrightarrow{m \rightarrow \infty} - \iint_{Q_T} r(c) \text{div}(\mathbf{V}) d\mathbf{x} dt = \iint_{Q_T} \nabla r(c) \cdot \mathbf{V} d\mathbf{x} dt,$$

so that $\mathbf{U} = \nabla r(c)$. \square

We have two kind of face values at hand : $(c_\sigma^n)_{\sigma \in \mathcal{E}_{\text{int}}, 1 \leq n \leq N}$ and $(\tilde{c}_\sigma^n)_{\sigma \in \mathcal{E}_{\text{int}}, 1 \leq n \leq N}$ defined respectively by (3.2) and (4.3). Based on this, we can reconstruct two approximate

concentration profiles $c_{\mathcal{E},\Delta t}$ and $\tilde{c}_{\mathcal{E},\Delta t}$ that are piecewise constant on the diamond cells by setting

$$c_{\mathcal{E},\Delta t}(t, \mathbf{x}) = \begin{cases} \mathcal{C}_\sigma^n & \text{if } (t, \mathbf{x}) \in (t_{n-1}, t_n] \times \Delta_\sigma, \quad \sigma \in \mathcal{E}_{\text{int}}, \\ c_K^n & \text{if } \mathbf{x} \in \Delta_\sigma, \quad \sigma \in \mathcal{E}_{\text{ext}} \cap \mathcal{E}_K, \end{cases} \quad (4.12) \quad \{\text{eq:c_Ee}\}$$

and

$$\tilde{c}_{\mathcal{E},\Delta t}(t, \mathbf{x}) = \begin{cases} \tilde{\mathcal{C}}_\sigma^n & \text{if } (t, \mathbf{x}) \in (t_{n-1}, t_n] \times \Delta_\sigma, \quad \sigma \in \mathcal{E}_{\text{int}}, \\ c_K^n & \text{if } \mathbf{x} \in \Delta_\sigma, \quad \sigma \in \mathcal{E}_{\text{ext}} \cap \mathcal{E}_K. \end{cases} \quad (4.13) \quad \{\text{eq:wt_c_E}\}$$

Lemma 4.2. *For the centered scheme and the Sedan scheme, there holds*

$$c_{\mathcal{E}_m, \Delta t_m} \xrightarrow{m \rightarrow \infty} c \quad \text{in } L^p(Q_T) \text{ for all } p \in [1, \infty), \quad (4.14) \quad \{\text{eq:conv_c}\}$$

$$\tilde{c}_{\mathcal{E}_m, \Delta t_m} \xrightarrow{m \rightarrow \infty} c \quad \text{in } L^p(Q_T) \text{ for all } p \in [1, \infty), \quad (4.15) \quad \{\text{eq:conv_w}\}$$

where c is as in Proposition 4.1.

Proof. We only prove (4.14) since the proof of (4.15) is similar. Here again, we get rid of m for clarity. Since $c_{\mathcal{T},\Delta t}$ converges almost everywhere to c and remains bounded between 0 and 1, it converges in $L^p(Q_T)$. $c_{\mathcal{E},\Delta t}$ is also uniformly bounded, hence it suffices to show that $\|c_{\mathcal{E},\Delta t} - c_{\mathcal{T},\Delta t}\|_{L^1(Q_T)}$ tends to 0. Denoting by $\Delta_{K\sigma}$ the half-diamond cell which is defined as the interior of the convex hull of $\{\mathbf{x}_K, \sigma\}$ for $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$, one has

$$\begin{aligned} \|c_{\mathcal{E},\Delta t} - c_{\mathcal{T},\Delta t}\|_{L^1(Q_T)} &\leq \sum_{n=1}^N \Delta t_n \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} m_{\Delta_{K\sigma}} |c_K^n - \mathcal{C}_\sigma^n| \\ &\leq \frac{h_{\mathcal{T}}}{d} \sum_{n=1}^N \Delta t_n \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} m_\sigma |c_K^n - \mathcal{C}_\sigma^n| \end{aligned}$$

where we have used the geometric relation $m(\Delta_{K\sigma}) = \frac{1}{d} m_\sigma \text{dist}(\mathbf{x}_K, \sigma) \leq \frac{h_{\mathcal{T}}}{d} m_\sigma$. For the internal faces, Lemma 3.1 (use (C.1) instead for $\tilde{\mathcal{C}}_\sigma^n$) implies that

$$|c_K^n - \mathcal{C}_\sigma^n| + |c_L^n - \mathcal{C}_\sigma^n| = |c_K^n - c_L^n|, \quad \forall \sigma = K|L.$$

Therefore, we obtain that

$$\begin{aligned} \|c_{\mathcal{E},\Delta t} - c_{\mathcal{T},\Delta t}\|_{L^1(Q_T)} &\leq \frac{h_{\mathcal{T}}}{d} \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} m_\sigma D_\sigma \mathbf{c}^n \\ &\leq \frac{h_{\mathcal{T}}}{d} \left(\sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} m_\sigma d_\sigma \right)^{1/2} \left(\sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}_{\text{int}}} \tau_\sigma |D_\sigma \mathbf{c}^n|^2 \right)^{1/2}. \end{aligned}$$

Since $|r(a) - r(b)| > |a - b|$ for all $a, b \in (0, 1)$, we deduce from Lemma 4.1 that

$$\|c_{\mathcal{E},\Delta t} - c_{\mathcal{T},\Delta t}\|_{L^1(Q_T)} \leq Ch_{\mathcal{T}}. \quad \square$$

c:identify

4.3. Convergence towards a weak solution.

Proposition 4.2. *Let c be as in Proposition 4.1 and let $\Phi \in L^\infty(Q_T) \cap L^\infty((0, T); H^1(\Omega))$ be the solution to the Poisson equation (1.3) with boundary conditions (1.6). Then, for the centered scheme and the Sedan scheme, there holds*

$$\pi_{\mathcal{T}_m, \Delta t_m} \Phi_m \xrightarrow{m \rightarrow \infty} \Phi \quad \text{in the } L^\infty(Q_T) \text{ weak-}\star \text{ sense,} \quad (4.16) \quad \{\text{eq:convPhi}\}$$

and

$$\nabla_{\mathcal{T}_m, \Delta t_m} \Phi_m \xrightarrow{m \rightarrow \infty} \nabla \Phi \quad \text{in the } L^\infty((0, T); L^2(\Omega)^d) \text{ weak-}\star \text{ sense.} \quad (4.17) \quad \{\text{eq:convPhi}\}$$

Proof. The existence of some $\Phi \in L^\infty(Q_T)$ such that (4.16) holds is a straightforward consequence of Lemma 3.4, whereas the existence of some $\mathbf{U} \in L^\infty((0, T); L^2(\Omega)^d)$ such that $\nabla_{\mathcal{T}_m, \Delta t_m} \Phi$ tends to \mathbf{U} as m tends to ∞ follows from Lemma 3.5 together with (4.1). The proof of $\mathbf{U} = \nabla \Phi$ is similar to the proof of Proposition 4.1.

We show now that Φ satisfies the Poisson equation (1.3). Let $\psi \in C_c^\infty([0, T] \times \{\Omega \cup \Gamma^N\})$, then define $\psi_K^n = \psi(\mathbf{x}_K, t_n)$ and $\psi_\sigma^n = \psi(\mathbf{x}_\sigma, t_n)$ for $1 \leq n \leq N$, $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_{\text{ext}}$. Following [21] (see [16] for a practical example), one can reconstruct a second approximate gradient operator $\widehat{\nabla}_{\mathcal{T}} : \mathbb{R}^{\mathcal{T}} \rightarrow L^\infty(\Omega)^d$ such that

$$\int_{\Omega} \nabla_{\mathcal{T}} \mathbf{u} \cdot \widehat{\nabla}_{\mathcal{T}} \mathbf{v} d\mathbf{x} = \sum_{\sigma \in \mathcal{E}} \tau_\sigma D_{K\sigma} \mathbf{u} D_{K\sigma} \mathbf{v}, \quad \forall \mathbf{u}, \mathbf{v} \in \mathbb{R}^{\mathcal{T}},$$

and which is strongly consistent, i.e.,

$$\widehat{\nabla}_{\mathcal{T}} \psi^n \xrightarrow{h_{\mathcal{T}} \rightarrow 0} \nabla \psi(\cdot, t_n) \text{ uniformly in } \overline{\Omega}, \quad \forall n \in \{1, \dots, N\}, \quad (4.18)$$

{eq:ov_gra

thanks to the smoothness of ψ . The scheme (2.4a) then reduces to

$$\int_{\Omega} \nabla_{\mathcal{T}} \Phi^n \cdot \widehat{\nabla}_{\mathcal{T}} \psi^n d\mathbf{x} = \int_{\Omega} \pi_{\mathcal{T}}(c^n + c^{dp}) \pi_{\mathcal{T}} \psi^n d\mathbf{x}, \quad \forall n \in \{1, \dots, N\}, \quad \forall \psi \in \mathbb{R}^{(\mathcal{T} + \mathcal{E}_{\text{ext}}) \times N}.$$

Integrating with respect to time over $(0, T)$ and passing to the limit $h_{\mathcal{T}}, \overline{\Delta t} \rightarrow 0$ thanks to Proposition 4.1, (4.17) and (4.18) then yields

$$\iint_{Q_T} \nabla \Phi \cdot \nabla \psi d\mathbf{x} dt = \iint_{Q_T} (c + c^{dp}) \psi d\mathbf{x} dt, \quad \forall \psi \in C_c^\infty([0, T] \times \Omega \cup \Gamma^N).$$

In particular, (1.15) holds for almost every $t \in (0, T)$.

The last point to be checked is the boundary condition for Φ , i.e., that $\Phi = \Phi^D$ on $(0, T) \times \Gamma^D$. This can be proved for instance following the lines of [7, Section 4]. \square

em:convPhi

Remark 4.2 (Enhanced convergence properties). The convergence described in Proposition 4.2 is not optimal. One can rather easily show that the convergence of $\pi_{\mathcal{T}_m, \Delta t_m} \Phi_m$ towards Φ for the strong topology of $L^2(Q_T)$ due to the strong convergence of $\pi_{\mathcal{T}_m, \Delta t_m} c_m$ to c established in Proposition 4.1. Moreover, one can establish the strong convergence of $\widehat{\nabla}_{\mathcal{T}_m, \Delta t_m} \Phi_m$ towards $\nabla \Phi$, where the gradient reconstruction operator $\widehat{\nabla}_{\mathcal{T}_m, \Delta t_m}$ is the extension to the time-space domain Q_T of the operator $\widehat{\nabla}_{\mathcal{T}_m}$ used in the proof of Proposition 4.2. We refer to [21] for details on these enhanced convergence properties.

prop:conv_c

Proposition 4.3. *Let c be as in Proposition 4.1, then c satisfies the weak formulation (1.14).*

Proof. Let $\varphi \in C_c^\infty([0, T] \times \overline{\Omega})$, then define $\varphi_K^n = \varphi(\mathbf{x}_K, t_n)$ for all $n \in \{0, \dots, N\}$ and $K \in \mathcal{T}$. Multiplying (2.4b) by $\Delta t_n \varphi_K^{n-1}$, then summing over $K \in \mathcal{T}$ and $n \in \{1, \dots, N\}$ and using expression (3.3) for the fluxes leads to

$$T_1 + T_2 + T_3 = 0, \quad (4.19)$$

{eq:T123}

where we have set

$$\begin{aligned} T_1 &= \sum_{n=1}^N \sum_{K \in \mathcal{T}} m_K (c_K^n - c_K^{n-1}) \varphi_K^{n-1}, \\ T_2 &= \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma \mathcal{C}_\sigma^n D_{K\sigma} h(\mathbf{c}^n) D_{K\sigma} \varphi^{n-1}, \\ T_3 &= \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma \mathcal{C}_\sigma^n D_{K\sigma} \Phi^n D_{K\sigma} \varphi^{n-1}. \end{aligned}$$

The term T_1 can be rewritten as

$$T_1 = \sum_{n=1}^N \Delta t_n \sum_{K \in \mathcal{T}} m_K c_K^n \frac{\varphi_K^{n-1} - \varphi_K^n}{\Delta t_n} - \sum_{K \in \mathcal{T}} m_K c_K^0 \varphi_K^0,$$

so that it follows from the convergence of $\pi_{\mathcal{T}, \Delta t} \mathbf{c}$ towards c and of $\pi_{\mathcal{T}} \mathbf{c}^0$ towards c^0 together with the regularity of φ that

$$T_1 \xrightarrow{m \rightarrow \infty} - \iint_{Q_T} c \partial_t \varphi d\mathbf{x} dt - \int_{\Omega} c^0 \varphi(0, \cdot) d\mathbf{x}. \quad (4.20) \quad \boxed{\text{eq:T1}}$$

On the other hand, the term T_3 can be rewritten as

$$T_3 = \iint_{Q_T} c_{\mathcal{E}, \Delta t} \nabla_{\mathcal{T}, \Delta t} \Phi \cdot \widehat{\nabla}_{\mathcal{T}, \Delta t} \varphi d\mathbf{x} dt,$$

where $\widehat{\nabla}_{\mathcal{T}, \Delta t}$ is the strongly consistent gradient reconstruction operator introduced in the proof of Proposition 4.2 and in Remark 4.2. In particular, due to the smoothness of φ , $\widehat{\nabla}_{\mathcal{T}, \Delta t} \varphi$ converges uniformly towards $\nabla \varphi$. Therefore, it follows from Lemma 4.2 and Proposition 4.2 that

$$T_3 \xrightarrow{m \rightarrow \infty} \iint_{Q_T} c \nabla \Phi \cdot \nabla \varphi d\mathbf{x} dt. \quad (4.21) \quad \boxed{\text{eq:T3}}$$

Define the term

$$\widetilde{T}_2 = \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma \widetilde{\mathcal{C}}_\sigma^n D_{K\sigma} h(\mathbf{c}^n) D_{K\sigma} \varphi^{n-1} = \iint_{Q_T} \nabla_{\mathcal{T}, \Delta t} r(\mathbf{c}) \cdot \widehat{\nabla}_{\mathcal{T}, \Delta t} \varphi d\mathbf{x} dt,$$

then it follows from Proposition 4.1 that

$$\widetilde{T}_2 \xrightarrow{m \rightarrow \infty} \iint_{Q_T} \nabla r(c) \cdot \nabla \varphi d\mathbf{x} dt.$$

Therefore, it only remains to show that $|T_2 - \widetilde{T}_2|$ tends to 0 to conclude the proof of Proposition 4.3. Thanks to the triangle and Cauchy-Schwarz inequalities, one has

$$\begin{aligned} |T_2 - \widetilde{T}_2| &\leq \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma \left| \mathcal{C}_\sigma^n - \widetilde{\mathcal{C}}_\sigma^n \right| D_\sigma h(\mathbf{c}^n) D_\sigma \varphi^{n-1} \\ &\leq \left(\sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma \mathcal{C}_\sigma^n |D_\sigma h(\mathbf{c}^n)|^2 \right)^{1/2} \left(\sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma \frac{(\mathcal{C}_\sigma^n - \widetilde{\mathcal{C}}_\sigma^n)^2}{\mathcal{C}_\sigma^n} |D_\sigma \varphi^{n-1}|^2 \right)^{1/2}. \end{aligned}$$

The first term in the right-hand side is uniformly bounded thanks to Remark 3.1, to $0 \leq \mathcal{C}_\sigma^n \leq 1$ and to Lemma 3.5 (we can adapt a part of the proof of (4.2)). Thus our

problem amounts to show that

$$\mathcal{R} := \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma \frac{(\mathcal{C}_\sigma^n - \tilde{\mathcal{C}}_\sigma^n)^2}{\mathcal{C}_\sigma^n} |D_\sigma \varphi^{n-1}|^2 \xrightarrow{m \rightarrow \infty} 0. \quad (4.22) \quad \boxed{\text{eq:Rto0}}$$

Let us reformulate \mathcal{R} as

$$\mathcal{R} := \sum_{n=1}^N \Delta t_n \sum_{\sigma \in \mathcal{E}} \tau_\sigma |\mathcal{C}_\sigma^n - \tilde{\mathcal{C}}_\sigma^n| \left| 1 - \frac{\tilde{\mathcal{C}}_\sigma^n}{\mathcal{C}_\sigma^n} \right| |D_\sigma \varphi^{n-1}|^2.$$

Thanks to (4.4), the quantity $\left| 1 - \frac{\tilde{\mathcal{C}}_\sigma^n}{\mathcal{C}_\sigma^n} \right|$ is uniformly bounded, whereas the regularity of φ implies that $D_\sigma \varphi^{n-1} \leq \|\nabla \varphi\|_\infty d_\sigma$. Putting this in the above expression of \mathcal{R} , we obtain that

$$\mathcal{R} \leq C \|c_{\mathcal{E}, \Delta t} - \tilde{c}_{\mathcal{E}, \Delta t}\|_{L^1(Q_T)} \xrightarrow{m \rightarrow \infty} 0,$$

thanks to Lemma 4.2. □

5. NUMERICAL COMPARISON OF THE SCHEMES

The numerical examples [29] have been implemented in the Julia language [5] based on the package `VoronoiFVM.jl` [30] which realizes the implicit Euler Voronoi finite volume method for nonlinear diffusion-convection-reaction equations on simplicial grids. The resulting nonlinear systems of equations are solved using Newton's method with parameter embedding. An advantage of the implementation in Julia is the availability of `ForwardDiff.jl` [40], an automatic differentiation package. This package allows the assembly of analytical Jacobians based on a generic implementation of nonlinear parameter functions without the need to write source code for derivatives.

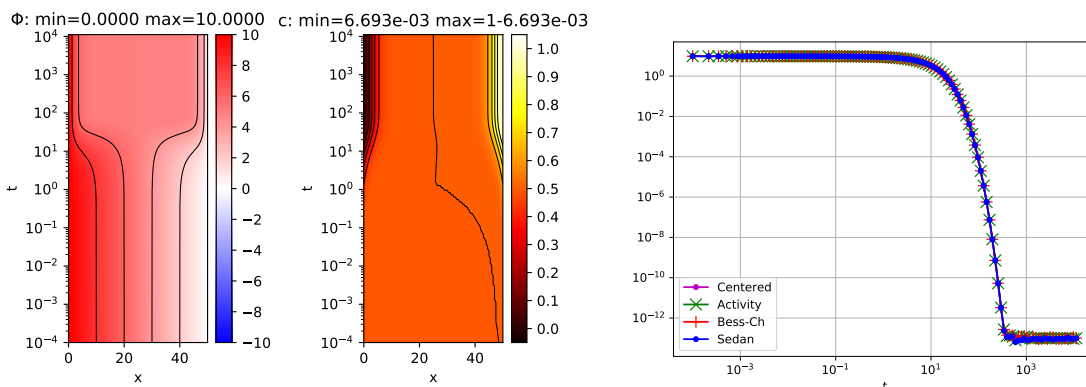


FIGURE 3. Left: time evolution of solution on domain $\Omega = (0, 50)$ from constant initial value $c = \frac{1}{2}$ with Dirichlet boundary conditions $\Phi(0) = 10$, $\Phi(50) = 0$, $c^{dp} = -\frac{1}{2}$ and homogeneous Neumann boundary conditions for c . Right: Evolution of the relative free energy according to (1.11). □

5.1. 1D time evolution and convergence test. The first group of examples considers the problem as described by (1.1)-(1.3) in a one-dimensional domain with Dirichlet boundary conditions for Φ and homogeneous Neumann boundary conditions for c . We regard the time evolution from a zero potential Φ and constant concentrations c_0 . In all examples we assume a constant doping concentration $c^{dp} = -\frac{1}{2}$. Calculations have been performed with subdivision of the domain $\Omega = (0, L)$ into 100 control volumes. Time steps have been chosen in a geometric progression $t_i = t_1 * \delta^i$ with $\delta = 1.15$ and $t_1 = 10^{-4}$.

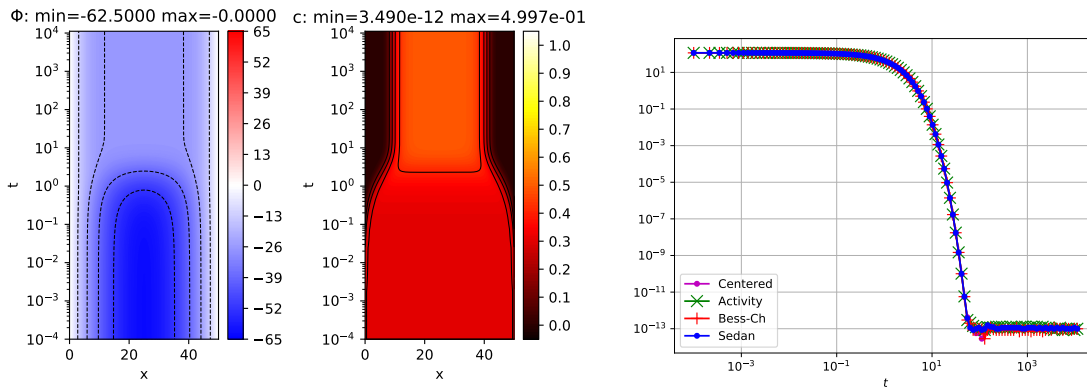


FIGURE 4. Left: time evolution of solution on domain $\Omega = (0, 50)$ from constant initial value $c = 0.3$ with Dirichlet boundary conditions $\Phi(0) = 0$, $\Phi(50) = 0$, $c^{dp} = -\frac{1}{2}$ and homogeneous Neumann boundary conditions for c . Right: Evolution of the relative free energy according to (1.11).

fig:evolii

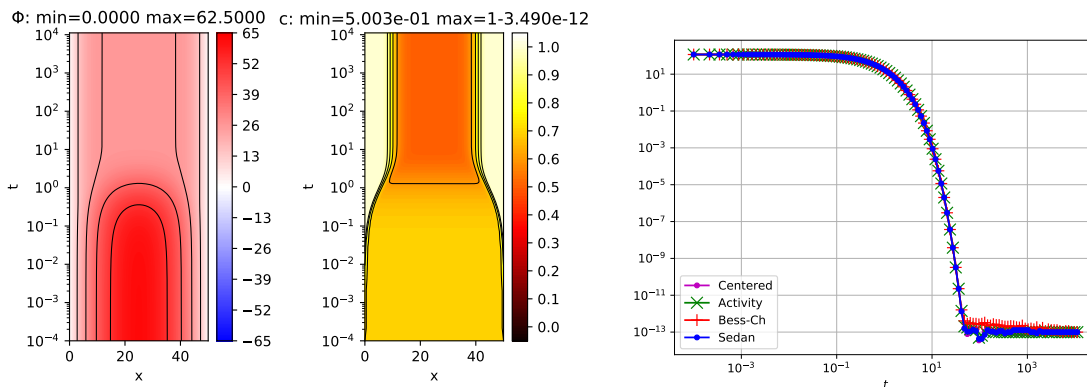


FIGURE 5. Left: time evolution of solution on domain $\Omega = (0, 50)$ from constant initial value $c = 0.7$ with Dirichlet boundary conditions $\Phi(0) = 0$, $\Phi(50) = 0$, $c^{dp} = -\frac{1}{2}$ and homogeneous Neumann boundary conditions for c . Right: Evolution of the relative free energy according to (1.11).

fig:evolii

In the first example (Fig. 3), $c_0 = 0.5$, and the initial amount of charge carriers exactly matches the amount of doping. With the start of time evolution, at $x = 0$ a potential of 10 is applied leading to a redistribution of the charge carrier concentration which for large t approaches a steady state with two space charge regions at the boundaries with opposite charge and an electroneutral region with $c = 0.5$ in the center of the domain. We remark, that the c stays in the range $(0, 1)$, and that the energy (1.11) decreases during time evolution for all four schemes discussed in this paper. We also remark that for zero applied potential, the constant values $\Phi = 0$ and $c = 0.5$ would comprise a solution for all $t > 0$.

Fig. 4 considers the case $c_0 = 0.3$. The available amount of charge carriers is not able to compensate the amount of doping. At the end of the time evolution, the charge carriers are concentrated in the center of the domain, establishing an electroneutral region. At both boundaries, depletion boundary layers create equally charged space charge regions due to the lack of charge carriers able to compensate the doping.

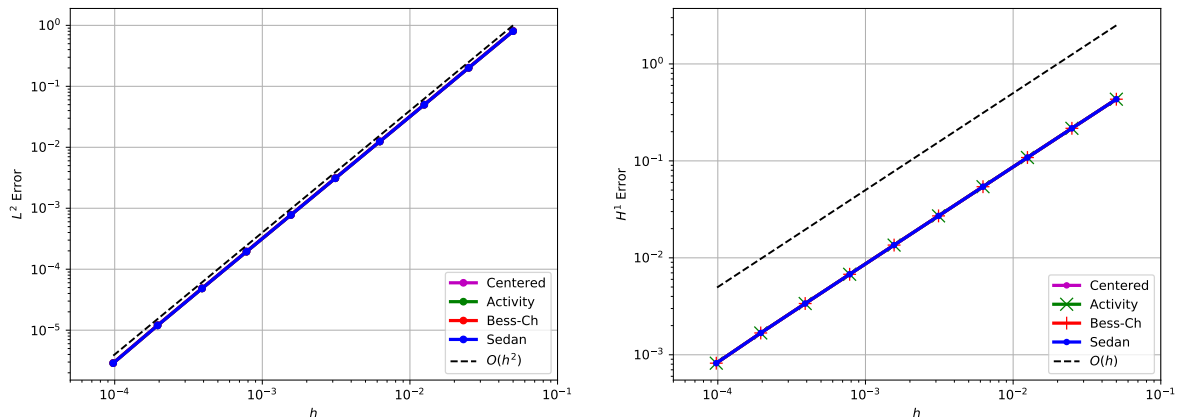


FIGURE 6. Convergence behavior of the different schemes for the case depicted in Fig. 3: comparison of solutions at $t = 10$. Left: L^2 -error, right: H^1 error. Correspondence to the equation in the paper: “Centered”: (2.8), “Sedan”: (2.9), “Activity”: (2.10), “Bess-Ch”: (2.11).

fig:scheme

Fig. 5 considers the case $c_0 = 0.7$ which in sense is symmetric to the previous one. There is again an electroneutral region in the center, and this time, “superfluous” charge carriers are forced to enrichment boundary layers.

Fig. 6 provides a comparison of the convergence behavior for the test case discussed in Fig. 3. We compare the solutions at a moment of time where we observe a rather large descent of the relative free energy based on a reference solution obtained on a fine grid of 40960 nodes. We observe first order convergence in the H^1 norm and second order convergence in the L^2 norm. No significant difference between the results for the various schemes.

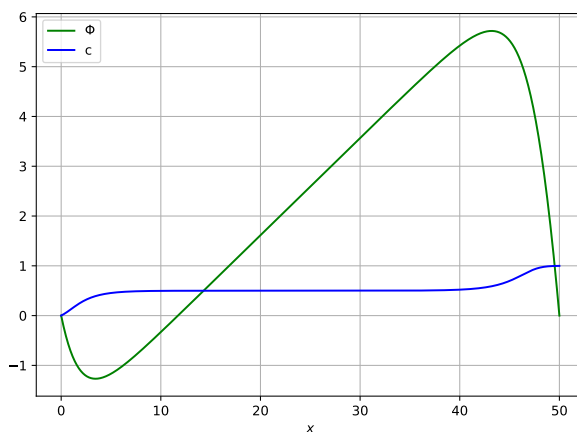


FIGURE 7. Stationary solution with Dirichlet boundary conditions for c and Φ .

fig:refsol

5.2. 1D stationary convergence test. In order to reveal the behavior of the various schemes under more extreme conditions, this convergence test outside of thermodynamic equilibrium includes regions of the solution with concentrations extremely close to 0 and 1, respectively, enforced by inhomogeneous Dirichlet boundary conditions for the concentration, thus leaving the realm of the analysis in this paper. Once again, we assume $\Omega = (0, L)$ with $L = 50$, $c^{dp} = -\frac{1}{2}$. We set boundary values $\Phi(0) = \Phi(L) = 0$ for the

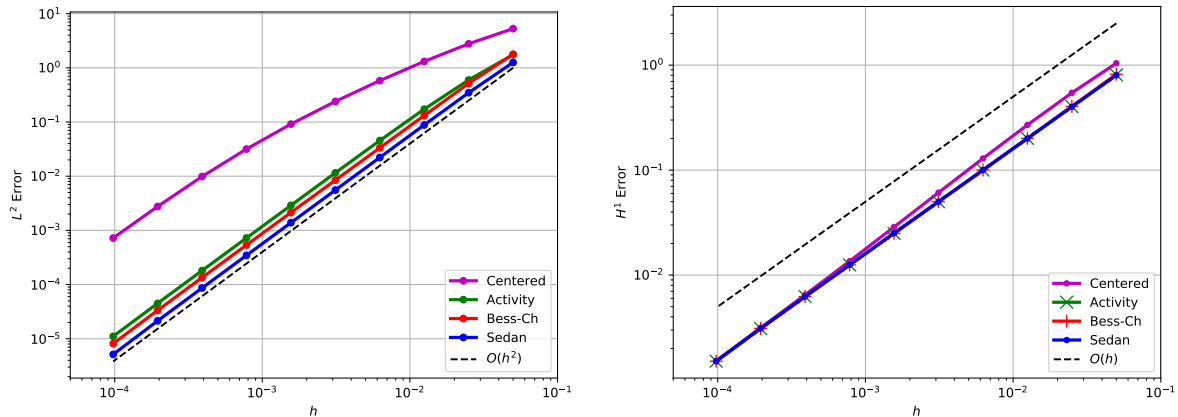


FIGURE 8. Convergence behavior of the different schemes. Left: L^2 -error, right: H^1 error. Correspondence to the equation in the paper: “Centered”: (2.8), “Sedan”: (2.9), “Activity”: (2.10), “Bess-Ch”: (2.11).

fig:scheme

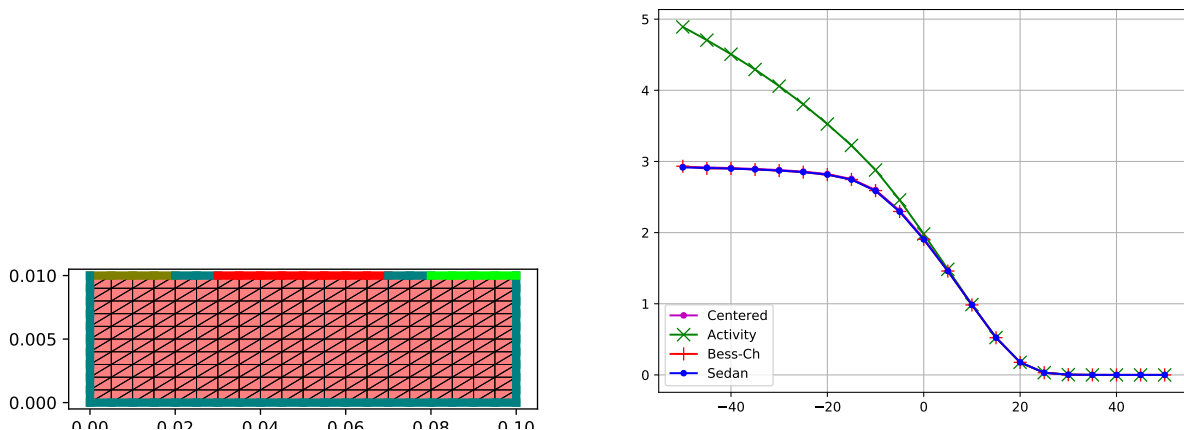


FIGURE 9. Discretization grid of refinement level $n_{ref} = 1$ (left) and corresponding I-V curves for different discretization schemes (right).

fig:gridiv

electrostatic potential, and $c(0) = 10^{-3}$, $c(L) = 1 - 10^{-3}$. We calculate a reference solution using the scheme (2.9) on a fine grid of 40960 nodes with grid spacing $h \simeq 1.22 \cdot 10^{-3}$, see Fig. 7. We use this solution as a surrogate for an analytical solution in a numerical investigation of the convergence rates of the different schemes. The result is shown in Fig. 8. We observe, that both in the H^1 and the L^2 norms, the schemes based on the modification of the Scharfetter-Gummel idea behave significantly better than the centered scheme. This is probably due to the Dirichlet boundary condition close to 0 where the function $c \mapsto h(c)$ appearing explicitly in the centered scheme is singular. Judging from the L^2 error plot in Fig. 8 (left), the scheme (2.9) converges better than all the others. Asymptotically, all schemes show the same standard behavior: we observe second order convergence in the L^2 norm and first order convergence in the H^1 -norm.

5.3. 2D Unipolar Field Effect Transistor. As a second example, we consider an unipolar field effect transistor. The domain is $\Omega = (0, L) \times (0, H)$ with $L = 10^{-2}$, $H =$

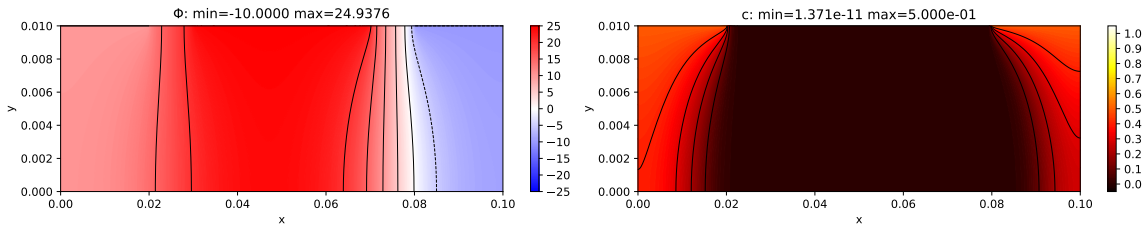


FIGURE 10. Electrostatic potential (left) and concentration (right) for closed gate ($U_{gate} = 50$).

fig:closed

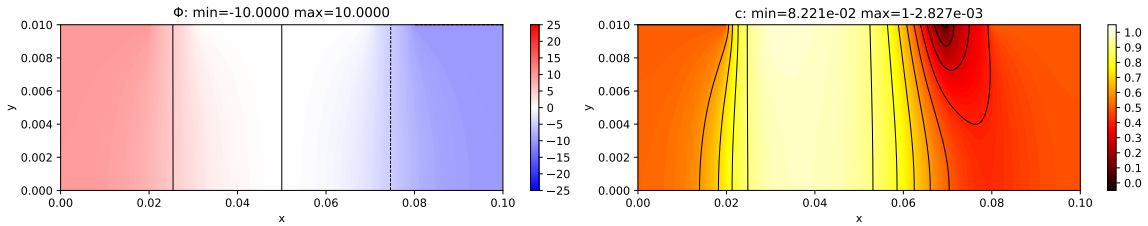


FIGURE 11. Electrostatic potential (left) and concentration (right) for $U_{gate} = 0$.

fig:g0

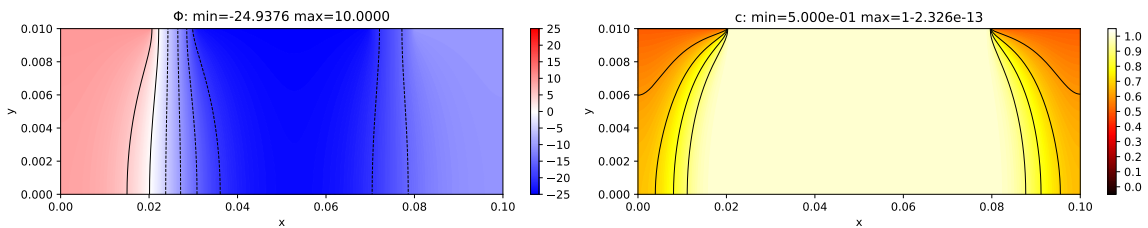


FIGURE 12. Electrostatic potential (left) and concentration (right) for open gate ($U_{gate} = -50$), with concentration in the channel reaching the saturation value 1.

fig:open

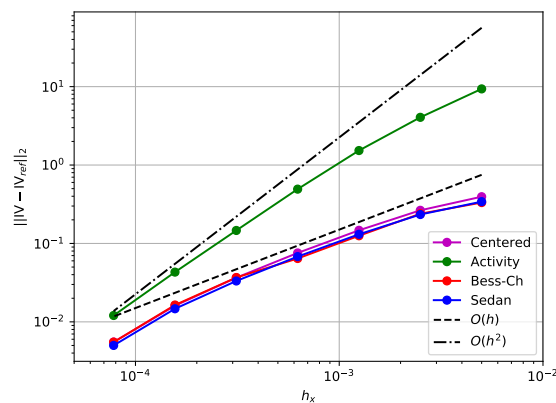


FIGURE 13. Convergence of the I-V curves calculated using the different discretization schemes.

fig:erriv

10^{-3} . We let $c^{dp} = -\frac{1}{2}$, and set the following boundary conditions at the contacts:

$$\begin{aligned} \begin{pmatrix} \Phi \\ c \end{pmatrix} &= \begin{pmatrix} -5 \\ \frac{1}{2} \end{pmatrix} \text{ at } \Gamma_{source} = (0, 0.2 \cdot L) \times H \\ \begin{pmatrix} \Phi \\ c \end{pmatrix} &= \begin{pmatrix} 5 \\ \frac{1}{2} \end{pmatrix} \text{ at } \Gamma_{drain} = (0.8 \cdot L, L) \times H \\ \begin{pmatrix} \nabla\Phi \cdot \mathbf{n} \\ \mathbf{J} \cdot \mathbf{n} \end{pmatrix} &= \begin{pmatrix} -\frac{1}{d}(\Phi - U_{gate}) \\ 0 \end{pmatrix} \text{ at } \Gamma_{gate} = (0.3 \cdot L, 0.7 \cdot L) \times H \\ \begin{pmatrix} \nabla\Phi \cdot \mathbf{n} \\ \mathbf{J} \cdot \mathbf{n} \end{pmatrix} &= \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ at } \partial\Omega \setminus (\Gamma_{gate} \cup \Gamma_{source} \cup \Gamma_{drain}). \end{aligned}$$

Here, $\Phi_{gate} \in (-50, 50)$ is the gate voltage, and $d = 0.1 \cdot H$ is the gate thickness. We introduce a slightly anisotropic rectangular grid $n_x \times n_y$ grid with $n_x = 10 \times 2^{n_{ref}}$ and $n_y = 5 \times 2^{n_{ref}}$, where n_{ref} is the refinement level. Each cell in the rectangular grid is subdivided into two triangles, see Fig. 9 (left). From the resulting triangle mesh, the Voronoi tessellation is obtained.

With fixed source and drain voltages, we vary the gate voltage U_{gate} from 50 to -50. At $U_{gate} = 50$, the positive applied potential pushes away the positively charged carriers from the channel – the region under the gate contact, see Fig. 10. The resulting lack of charge carriers results in a near zero current. With decreasing gate voltage, more and more charge carriers are allowed into the channel, leading to an increase in the current. When the gate voltage decreases further, charge carriers are attracted to the gate contact and fill up the channel. Due to the degeneration, their concentration cannot exceed 1. As a result, we observe a saturation of the current close to some maximum value for gate voltages approaching -50, see Fig. 10.

All schemes under consideration with the exception of (2.10) represent this saturation behaviour quite well already at rather coarse grids, see Fig. 9 (right). This appears to be in line with earlier investigations of the scheme based on activity averaging [26] which hint that its asymptotic behavior for large electric fields is not satisfactory.

In order to get an idea about the convergence in this case, we produce a reference solution on a grid with 821121 nodes using the scheme (2.9) and compare the calculated I-V curves. The behavior of the error in the I-V curves is shown in Fig. 13. While all four schemes exhibit convergence of order at least $O(h)$, the activity based scheme (2.10) converges with a constant approximately one order of magnitude larger than the others.

APPENDIX A. L^∞ BOUND ON THE TPFA FV APPROXIMATE POISSON EQUATION

It is well know that the solution to the Poisson equation

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = u^D & \text{on } \Gamma^D, \\ \nabla u \cdot \mathbf{n} = 0 & \text{on } \Gamma^N, \end{cases} \quad (\text{A.1})$$

is bounded in $L^\infty(\Omega)$ provided $f \in L^\infty(\Omega)$ and $u^D \in L^\infty(\partial\Omega)$. The goal of this appendix is to get a discrete counterpart of this estimate for TPFA finite volume approximations of (A.1). The data u^D and f are discretized into

$$u_\sigma^D = \frac{1}{m_\sigma} \int_\sigma u^D(\boldsymbol{\gamma}) d\boldsymbol{\gamma}, \quad f_K = \frac{1}{m_K} \int_K f d\mathbf{x}, \quad \sigma \in \mathcal{E}^D, K \in \mathcal{T}.$$

and the classical TPFA finite volume scheme writes:

$$-\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K\sigma} u = m_K f_K, \quad \forall K \in \mathcal{T}.$$

The associate linear system of equations can be written as

$$\mathbb{L} \mathbf{u} = \mathbf{b}, \quad (\text{A.2})$$

with $\mathbf{u} = (u_K, u_\sigma)_{K \in \mathcal{T}, \sigma \in \mathcal{E}^D}$ (let us note that we keep the Dirichlet nodes in the set of unknowns), $\mathbf{b} = (f_K, u_\sigma^D)_{K \in \mathcal{T}, \sigma \in \mathcal{E}^D}$ and $\mathbb{L} \in \mathbb{R}^{(\mathcal{T} + \mathcal{E}^D) \times (\mathcal{T} + \mathcal{E}^D)}$ is the sparse symmetric definite positive matrix defined by

$$\begin{aligned} \mathbb{L}_{\sigma, \sigma} &= 1, & \mathbb{L}_{\sigma, \ell} &= 0 \text{ if } \ell \neq \sigma, & \sigma &\in \mathcal{E}^D, \\ \mathbb{L}_{K, K\sigma} &= -\frac{\tau_\sigma}{m_K}, & \mathbb{L}_{K, K} &= \frac{1}{m_K} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma, & K &\in \mathcal{T}. \end{aligned}$$

In the above definition of \mathbb{L} , ℓ denotes an arbitrary index in $\mathcal{T} \cup \mathcal{E}^D$, whereas $K\sigma$ denotes the mirror index of K w.r.t. the faces $\sigma \in \mathcal{E}_K$, i.e., $K\sigma = L$ if $\sigma = K|L \in \mathcal{E}_K \cap \mathcal{E}_{\text{int}}$ and $K\sigma = \sigma$ if $\sigma \in \mathcal{E}_K \cap \mathcal{E}^D$.

The goal of this section is to derive an ℓ^∞ bound on the solution \mathbf{u} to the linear system (A.2) which is uniform w.r.t. the mesh. This is the purpose of the following proposition.

Proposition A.1. *There exists C depending only on Ω such that*

$$|u_K| \leq C \max \{ \|u^D\|_{L^\infty(\partial\Omega)}, \|f\|_{L^\infty(\Omega)} \}, \quad \forall K \in \mathcal{T}.$$

Proof. The proof we propose here is an extension to the context of TPFA Finite Volumes of the proof of Hackbusch [35] for Finite Differences. An alternative proof of Proposition A.1 based on Stampacchia's truncation estimates is sketched in [32].

The definitions of u_σ^D and f_K ensure that

$$\|\mathbf{b}\|_\infty \leq \max \{ \|u^D\|_{L^\infty(\partial\Omega)}, \|f\|_{L^\infty(\Omega)} \},$$

so that

$$\|\mathbf{u}\|_\infty \leq \|\mathbb{L}^{-1}\|_\infty \|\mathbf{b}\|_\infty \leq \|\mathbb{L}^{-1}\|_\infty \max \{ \|u^D\|_{L^\infty(\partial\Omega)}, \|f\|_{L^\infty(\Omega)} \}.$$

Therefore, it only remains to check that $\|\mathbb{L}^{-1}\|_\infty \leq C$ for some C not depending on \mathcal{T} .

The matrix \mathbb{L} is a M -matrix (see [35, Definition 4.8]). Therefore, owing to [35, Theorem 4.24], if we can exhibit some vector $\mathbf{w} \in \mathbb{R}^{\mathcal{T} + \mathcal{E}^D}$ such that $\mathbb{L}\mathbf{w} \geq \mathbf{1}$, then $\|\mathbb{L}^{-1}\|_\infty \leq \|\mathbf{w}\|_\infty$. Define the function $w : \bar{\Omega} \rightarrow \mathbb{R}$ by

$$w(\mathbf{x}) = 1 + \frac{1}{d} \left(\sup_{\mathbf{y} \in \Omega} |\mathbf{y}|^2 - |\mathbf{x}|^2 \right) \geq 1, \quad \mathbf{x} \in \bar{\Omega},$$

and the vector $\mathbf{w} = (w_K, w_\sigma)$ by $w_K = w(\mathbf{x}_K)$, $K \in \mathcal{T}$, and $w_\sigma = w(\mathbf{x}_\sigma)$, $\sigma \in \mathcal{E}^D$.

The estimate on the Dirichlet nodes is straightforward:

$$(\mathbb{L}\mathbf{w})_\sigma = w_\sigma \geq 1, \quad \forall \sigma \in \mathcal{E}^D.$$

Now, let us focus on the inner nodes $K \in \mathcal{T}$. Since $\sum_{\ell \in \mathcal{T} \cup \mathcal{E}^D} \mathbb{L}_{K,\ell} = \sum_{\sigma \in \mathcal{E}_K} \mathbb{L}_{K,K\sigma} = 0$, one has

$$\begin{aligned} (\mathbb{L}\mathbf{w})_K &= \frac{1}{d} \sum_{\sigma \in \mathcal{E}_K} \mathbb{L}_{K,K\sigma} |\mathbf{x}_{K\sigma}|^2 = \frac{1}{dm_K} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma (|\mathbf{x}_K|^2 - |\mathbf{x}_{K\sigma}|^2) \\ &= \frac{1}{dm_K} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma (|\mathbf{x}_K - \mathbf{x}_{K\sigma}|^2 + 2\mathbf{x}_K \cdot (\mathbf{x}_K - \mathbf{x}_{K\sigma})) \\ &= \frac{1}{dm_K} \sum_{\sigma \in \mathcal{E}_K} m_\sigma d_\sigma + \frac{2}{dm_K} \mathbf{x}_K \cdot \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma (\mathbf{x}_K - \mathbf{x}_{K\sigma}). \end{aligned}$$

Because of the geometric relation $m_\sigma d_\sigma = dm_{\Delta_\sigma}$, and since $K \subset \bigcup_{\sigma \in \mathcal{E}_K} \Delta_\sigma$, there holds

$$\frac{1}{dm_K} \sum_{\sigma \in \mathcal{E}_K} m_\sigma d_\sigma = \frac{1}{m_K} \sum_{\sigma \in \mathcal{E}_K} m_{\Delta_\sigma} \geq 1.$$

On the other hand, the second term vanishes since

$$\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma (\mathbf{x}_K - \mathbf{x}_{K\sigma}) = - \sum_{\sigma \in \mathcal{E}_K} m_\sigma \mathbf{n}_{K\sigma} = \mathbf{0}.$$

Therefore, $(\mathbb{L}\mathbf{w})_K \geq 1$ for all $K \in \mathcal{T}$. As a consequence,

$$\|\mathbb{L}^{-1}\|_\infty \leq \|\mathbf{w}\|_\infty = 1 + \frac{1}{d} \sup_{\mathbf{y} \in \Omega} |\mathbf{y}|^2 \leq 1 + \frac{\text{diam}(\Omega)^2}{4d}.$$

The last estimate comes from the fact that one can choose the origin for \mathbf{y} arbitrarily. \square

APPENDIX B. PROOF OF LEMMA 3.2

Step 1. Let $\delta \in (0, 1)$ and $M \in \mathbb{R}$. We start with the proof of

$$\lim_{c_L \rightarrow 1} \Upsilon_{\delta, M}(c_L) = +\infty \tag{B.1} \quad \boxed{\text{lim_Upsilon1}}$$

where

$$\Upsilon_{\delta, M}(c_L) = \inf \left\{ \mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in (0, 1 - \delta], (\Phi_K, \Phi_L) \in [-M, M]^2 \right\}.$$

We recall that

$$\begin{aligned} \mathcal{D}(c_K, c_L, \Phi_K, \Phi_L) &= \mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) |h(c_K) + \Phi_K - h(c_L) - \Phi_L|^2, \\ &= \mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) (h(c_K) + \Phi_K - h(c_L) - \Phi_L) \end{aligned}$$

and we notice that the diffusion force blows up:

$$\liminf_{c_L \rightarrow 1} \left\{ |h(c_K) - h(c_L) + \Phi_K - \Phi_L|; c_K \in (0, 1 - \delta], (\Phi_K, \Phi_L) \in [-M, M]^2 \right\} = +\infty. \tag{B.2} \quad \boxed{\text{eq:diff-f}}$$

Therefore, we can get (B.1) by proving that either $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L)$ or $\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L)$ stays bounded away from 0, uniformly in $c_K \in (0, 1 - \delta]$, $(\Phi_K, \Phi_L) \in [-M, M]^2$, for $c_L \geq 1/2$.

For the centered flux, we have that, for all $(c_K, \Phi_K, \Phi_L) \in (0, 1 - \delta] \times [-M, M]^2$, $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = (c_K + c_L)/2 \geq c_L/2$. This yields (B.1). For the three other schemes, we remark that, for any $\alpha \in (0, 1 - \delta)$, we can rewrite

$$\Upsilon_{\delta, M}(c_L) = \min(\Upsilon_{\delta, M}^{\alpha, 1}(c_L), \Upsilon_{\delta, M}^{\alpha, 2}(c_L)),$$

where

$$\begin{aligned}\Upsilon_{\delta,M}^{\alpha,1}(c_L) &= \inf \{ \mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in (0, \alpha), (\Phi_K, \Phi_L) \in [-M, M]^2 \} \\ \Upsilon_{\delta,M}^{\alpha,2}(c_L) &= \inf \{ \mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in [\alpha, 1 - \delta], (\Phi_K, \Phi_L) \in [-M, M]^2 \}\end{aligned}$$

But Lemma 3.1 ensures that, independently of the choice of the numerical flux, we have at least $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) \geq \min(c_K, c_L)/2$, so that $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) \geq \alpha/2$ for all $(c_K, c_L, \Phi_K, \Phi_L) \in [\alpha, 1 - \delta] \times [1/2, 1) \times [-M, M]^2$ if $\alpha \in (0, 1 - \delta)$. Therefore, for all $\alpha \in (0, 1 - \delta)$, we have

$$\lim_{c_L \rightarrow 1} \Upsilon_{\delta,M}^{\alpha,2}(c_L) = +\infty.$$

It remains to prove that for a given $\alpha \in (0, 1 - \delta)$ we also have

$$\lim_{c_L \rightarrow 1} \Upsilon_{\delta,M}^{\alpha,1}(c_L) = +\infty. \quad (\text{B.3})$$

{lim_Upsi1}

Because of the monotonicity of $\delta \mapsto \Upsilon_{\delta,M}(c_L)$, we can restrict our attention to the case $\delta \leq 1/2$, so that we can seek for $\alpha \in (0, 1/2]$.

For the Bessemoulin-Chatard flux, we have

$$\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) = dr(c_K, c_L) \left\{ B \left(\frac{\Phi_L - \Phi_K}{dr(c_K, c_L)} \right) c_K - B \left(\frac{\Phi_K - \Phi_L}{dr(c_K, c_L)} \right) c_L \right\},$$

with $dr(c_K, c_L) \geq 1$. Using the monotonicity of the Bernoulli function and the bounds on Φ_K and Φ_L , we get:

$$B(2M) \leq B \left(\pm \frac{\Phi_L - \Phi_K}{dr(c_K, c_L)} \right) \leq B(-2M)$$

Hence, for $\alpha = \frac{B(2M)}{4B(-2M)}$:

$$\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) \leq dr(c_K, c_L) \left\{ B(-2M)\alpha - B(2M)\frac{1}{2} \right\} \leq -\frac{B(2M)}{4}$$

Then, thanks to (B.2), we deduce (B.3) for $\alpha = \frac{B(2M)}{4B(-2M)}$ and therefore (B.1).

For the Sedan flux, we use similarly the monotonicity of the function B and ν , so that

$$\begin{aligned}\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) &\leq B \left(-2M + \nu\left(\frac{1}{2}\right) - \nu(\alpha) \right) \alpha - B \left(2M - \nu\left(\frac{1}{2}\right) + \nu(\alpha) \right) \frac{1}{2} \\ &\quad \forall c_K \in (0, \alpha), c_L \in \left(\frac{1}{2}, 1\right), (\Phi_K, \Phi_L) \in [-M, M]^2.\end{aligned}$$

But the right-hand-side of the last inequality has a negative limit when α tends to 0, which means that for a given α small enough it remains bounded away from 0, so that we deduce (B.3) and therefore (B.1).

For the activity based flux, we also use the monotonicity of a and β , which yields

$$\begin{aligned}\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) &\leq \frac{1}{4} \left(B(-2M)a(\alpha) - B(2M)a\left(\frac{1}{2}\right) \right) \\ &\quad \forall c_K \in (0, \alpha), c_L \in \left(\frac{1}{2}, 1\right), (\Phi_K, \Phi_L) \in [-M, M]^2.\end{aligned}$$

The right-hand-side has a negative limit when α tends to 0. Thus it remains bounded away from 0 for a given $\alpha < 1/2$ and we deduce (B.3) and therefore (B.1).

Step 2. We now focus on the proof of

$$\lim_{c_L \rightarrow 0} \Psi_{\delta,M}(c_L) = +\infty \quad (\text{B.4})$$

{lim_Psi}

where

$$\Psi_{\delta,M}(c_L) = \inf \left\{ \mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in [\delta, 1), (\Phi_K, \Phi_L) \in [-M, M]^2 \right\}.$$

We use similar arguments than in Step 1. First, the diffusion force still blows up :

$$\liminf_{c_L \rightarrow 0} \left\{ \left| h(c_K) - h(c_L) + \Phi_K - \Phi_L \right|; c_K \in [\delta, 1), (\Phi_K, \Phi_L) \in [-M, M]^2 \right\} = +\infty. \quad (\text{B.5})$$

{eq:diff-f

For the centered flux, we have : $\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = (c_K + c_L)/2 \geq \delta/2$ hence (B.4). For the other fluxes, we rewrite again

$$\Psi_{\delta,M}(c_L) = \min(\Psi_{\delta,M}^{\alpha,1}(c_L), \Psi_{\delta,M}^{\alpha,2}(c_L)),$$

where

$$\Psi_{\delta,M}^{\alpha,1}(c_L) = \inf \left\{ \mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in [\delta, \alpha], (\Phi_K, \Phi_L) \in [-M, M]^2 \right\};$$

$$\Psi_{\delta,M}^{\alpha,2}(c_L) = \inf \left\{ \mathcal{D}(c_K, c_L, \Phi_K, \Phi_L); c_K \in (\alpha, 1), (\Phi_K, \Phi_L) \in [-M, M]^2 \right\}.$$

Using the symmetry of the flux $\mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) = -\mathcal{F}(c_L, c_K, \Phi_L, \Phi_K)$ and following the proof of (B.3), we get that for $\alpha = 1/2$,

$$\lim_{c_L \rightarrow 0} \Psi_{\delta,M}^{\alpha,2}(c_L) = +\infty$$

We now have to prove that, for $\alpha = 1/2$,

$$\lim_{c_L \rightarrow 0} \Psi_{\delta,M}^{\alpha,1}(c_L) = +\infty \quad (\text{B.6})$$

{lim_Psi_a

To this end, we will show bounds on the flux. The set $[\delta, \alpha] \times [-M, M]^2$ is compact, and the flux functions are continuous. It is sufficient to show a positive lower bound for the limit at any $(c^*, \Phi^*, \Phi_*) \in [\delta, \alpha] \times [-M, M]^2$:

$$l^* = \lim_{(c_K, c_L, \Phi_K, \Phi_L) \rightarrow (c^*, 0, \Phi^*, \Phi_*)} \mathcal{F}(c_K, c_L, \Phi_K, \Phi_L) > 0.$$

For the Sedan scheme, we have:

$$l^* = B(\Phi_* - \Phi^* - \nu(c^*))c^* \geq \delta B(2M).$$

For the Bessemoulin-Chatard scheme, we have: $\lim_{(c_K, c_L) \rightarrow (c^*, 0)} dr(c_K, c_L) = 1$, hence:

$$l^* = B(\Phi_* - \Phi^*)c^* \geq \delta B(2M).$$

For the activity based scheme we have:

$$l^* = \frac{\beta(c^*) + 1}{2} B(\Phi_* - \Phi^*)a(c^*) \geq \frac{a(\delta)}{2} B(2M).$$

As these limits are bounded away from zero we have (B.6) hence (B.4). It concludes the proof of Lemma 3.2.

APPENDIX C. COMPARISON OF FACE CONCENTRATION FUNCTIONALS

For each scheme, we have defined a face concentration functional $\mathcal{C} : (0, 1) \times (0, 1) \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$. We introduce a second face concentration functional $\tilde{\mathcal{C}} : (0, 1) \times (0, 1) \rightarrow \mathbb{R}$, defined by

$$\tilde{\mathcal{C}}(c_K, c_L) = \frac{r(c_K) - r(c_L)}{h(c_K) - h(c_L)} \text{ if } c_K \neq c_L \text{ and } c_K \text{ otherwise.}$$

As $r'(c) = ch'(c)$, it is clear that

$$\min(c_K, c_L) \leq \tilde{\mathcal{C}}(c_K, c_L) \leq \max(c_K, c_L) \text{ for all } (c_K, c_L) \in (0, 1) \times (0, 1). \quad (\text{C.1})$$

{eq:wt_avg

Lemma C.1 states a comparison between \mathcal{C} and $\tilde{\mathcal{C}}$ for the centered and the Sedan schemes.

Lemma C.1. *For the centered scheme and the Sedan scheme, there exists $G > 0$, depending only on M , such that for all $(c_K, c_L, \Phi_K, \Phi_L) \in (0, 1) \times (0, 1) \times [-M, M] \times [-M, M]$,*

$$\frac{\tilde{\mathcal{C}}(c_K, c_L)}{\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L)} \leq G. \quad (\text{C.2})$$

Proof. The case of the centered scheme defined by (2.8) is the easiest one, since

$$\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L) = \frac{c_K + c_L}{2} \geq \frac{1}{2} \max(c_K, c_L),$$

so that (C.2) holds with $G = 2$ thanks to (C.1).

Let us now focus on the Sedan scheme defined by (2.9). We can introduce the function $\mathcal{G} : (0, 1) \times (0, 1) \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ defined by

$$\mathcal{G}(c_K, c_L, \Phi_K, \Phi_L) = \frac{\tilde{\mathcal{C}}(c_K, c_L)}{\mathcal{C}(c_K, c_L, \Phi_K, \Phi_L)}.$$

It is a continuous function which satisfies the symmetry property $\mathcal{G}(c_K, c_L, \Phi_K, \Phi_L) = \mathcal{G}(c_L, c_K, \Phi_L, \Phi_K)$ and the consistency $\mathcal{G}(c_K, c_K, \Phi_K, \Phi_L) = 1$. Bearing in mind the expression (3.12) of \mathcal{C} , with $x = \log(c_K) - \log(c_L)$, $y = \Phi_L + \nu(c_L) - \Phi_K - \nu(c_K)$ and $x - y = h(c_K) + \Phi_K - h(c_L) - \Phi_L$, one can rewrite

$$\mathcal{G}(c_K, c_L, \Phi_K, \Phi_L) = \frac{(h(c_K) + \Phi_K - h(c_L) - \Phi_L)(r(c_K) - r(c_L))}{(B(y)c_K - B(-y)c_L)(h(c_K) - h(c_L))}$$

Because of the symmetry and the consistency properties, we can assume without loss of generality that $c_K > c_L$. Using the average properties (3.7) and (C.1), one obtains that

$$\mathcal{G}(c_K, c_L, \Phi_K, \Phi_L) \leq \frac{c_K}{c_L} \leq \frac{1}{c_L}, \quad (\text{C.3})$$

so that we only have to check that $\mathcal{G}(c_K, c_L, \Phi_K, \Phi_L)$ remains uniformly bounded as c_L tends to 0 in order to prove (C.2). Therefore, considering that (Φ_K, Φ_L) is given, we study the limit of \mathcal{G} when (c_K, c_L) tends to $(1, 0)$, $(0, 0)$ and $(c^*, 0)$ with $c^* \in (0, 1)$.

We first consider the limit $(c_K, c_L) \rightarrow (1, 0)$. We have the following equivalences when $(c_K, c_L) \rightarrow (1, 0)$:

$$\begin{aligned} h(c_K) - h(c_L) &\sim -\log(1 - c_K) - \log(c_L) \\ h(c_K) + \Phi_K - h(c_L) - \Phi_L &\sim -\log(1 - c_K) - \log(c_L) \\ r(c_K) - r(c_L) &\sim -\log(1 - c_K) \\ B(y)c_K - B(-y)c_L &\sim -c_K \log(1 - c_K) \end{aligned}$$

This yields:

$$\lim_{(c_K, c_L) \rightarrow (1, 0)} \mathcal{G}(c_K, c_L, \Phi_K, \Phi_L) = 1 \quad \forall (\Phi_K, \Phi_L) \in \mathbb{R} \times \mathbb{R}. \quad (\text{C.4})$$

With similar arguments, we compute the limit $(c_K, c_L) \rightarrow (c^*, 0)$ with $c^* \in (0, 1)$. We get:

$$\lim_{(c_K, c_L) \rightarrow (c^*, 0)} \mathcal{G}(c_K, c_L, \Phi_K, \Phi_L) = \frac{r(c^*)}{B(y^*)c^*} \quad \forall (\Phi_K, \Phi_L) \in \mathbb{R} \times \mathbb{R}, \quad (\text{C.5})$$

with $y^* = \Phi_L - \Phi_K + \log(1 - c^*)$.

In the neighborhood of $(0, 0)$, the behaviour is more complex, as the limit of $\log(c_K/c_L)$ is not defined and \mathcal{G} does not have a limit. However, thanks to C.3, $\mathcal{G}(c_K, c_L, \Phi_K, \Phi_L)$

stays bounded if c_K/c_L stays bounded while $(c_K, c_L) \rightarrow (0, 0)$. It remains to consider the case where $(c_K, c_L) \rightarrow (0, 0)$ while $c_K/c_L \rightarrow \infty$. In this case,

$$\begin{aligned} \frac{(h(c_K) + \Phi_K - h(c_L) - \Phi_L)}{h(c_K) - h(c_L)} &\rightarrow 1, \\ r(c_K) - r(c_L) &\sim -c_L + c_K \\ B(y)c_K - B(-y)c_L &\sim B(\Phi_L - \Phi_K)c_K - B(\Phi_K - \Phi_L)c_L, \end{aligned}$$

and

$$\lim_{\substack{(c_K, c_L) \rightarrow (0, 0) \\ c_K/c_L \rightarrow \infty}} \mathcal{G}(c_K, c_L, \Phi_K, \Phi_L) = \frac{1}{B(\Phi_L - \Phi_K)}.$$

We conclude that $\mathcal{G}(c_K, c_L, \Phi_K, \Phi_L)$ stays bounded when (c_K, c_L) is in the neighborhood of $(0, 0)$ for all $(\Phi_K, \Phi_L) \in \mathbb{R}^2$. Combined with (C.3), (C.4) and (C.5), it concludes the proof of Lemma C.1. \square

Remark C.1. For the Bessemoulin-Chatard scheme, the bound (C.2) does not hold. Let us consider that $\Phi_K = \Phi_L = \Phi$, then with the notations $x = \log(c_K/c_L)$, and $y = \log(\frac{1-c_L}{1-c_K})$, we have:

$$\frac{\tilde{\mathcal{C}}(c_K, c_L)}{\mathcal{C}(c_K, c_L, \Phi, \Phi)} = \frac{xy}{(c_K - c_L)(x + y)}.$$

For $(c_K, c_L) \rightarrow (1, 0)$, x and y tends to $+\infty$, hence the blow up of the ratio.

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CLÉMENT CANCÈS: INRIA, UNIV. LILLE, CNRS, UMR 8524 - LABORATOIRE PAUL PAINLEVÉ, F-59000 LILLE (clement.cances@inria.fr)

CLAIRE CHAINAIS-HILLAIRET: UNIV. LILLE, CNRS, UMR 8524, INRIA - LABORATOIRE PAUL PAINLEVÉ, F-59000 LILLE (claire.chanais@univ-lille.fr)

JÜRGEN FUHRMANN: WEIERSTRASS INSTITUTE (WIAS), MOHRENSTR. 39, 10117 BERLIN, GERMANY (juergen.fuhrmann@wias-berlin.de)

BENOÎT GAUDEUL: UNIV. LILLE, CNRS, UMR 8524, INRIA - LABORATOIRE PAUL PAINLEVÉ, F-59000 LILLE (benoit.gaudeul@univ-lille.fr)