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A POSITIVE CELL VERTEX GODUNOV SCHEME FOR A BEELER-REUTER BASED MODEL OF CARDIAC ELECTRICAL ACTIVITY

MOSTAFA BENDAHMANE, FATIMA MROUÉ, AND MAZEN SAAD

ABSTRACT. The monodomain model is a widely used model in electrocardiology to simulate the propagation of electrical potential in the myocardium. In this paper, we investigate a positive nonlinear control volume finite element (CVFE) scheme, based on Godunov's flux approximation of the diffusion term, for the monodomain model coupled to a physiological ionic model (the Beeler-Reuter model) and using an anisotropic diffusion tensor. In this scheme, degrees of freedom are assigned to vertices of a primal triangular mesh, as in conforming finite element methods. The diffusion term which involves an anisotropic tensor is discretized on a dual mesh using the diffusion fluxes provided by the conforming finite element reconstruction on the primal mesh and the other terms are discretized by means of an upwind finite volume method on the dual mesh. The scheme ensures the validity of the discrete maximum principle without any restriction on the transmissibility coefficients. By using a compactness argument, we obtain the convergence of the discrete solution and as a consequence, we get the existence of a weak solution of the original model. Finally, we illustrate the efficiency of the proposed scheme by exhibiting some numerical results.

Keywords: Monodomain model, Finite volume, Finite Element, Godunov Scheme, Maximum principle, Convergence

1. Introduction

Recent electrocardiology studies consider the bidomain model, that was introduced in the pioneering work [32], as the most accurate and physiologically based model describing cardiac electrical activity [15, 33, 24]. In this model, the anisotropic cardiac tissue is represented by averaging electric properties over a length scale greater than that of a single cell. We refer to [24] for a derivation of the bidomain equations, to [27, 29] for detailed reviews and to [8] for a rigourous derivation of the bidomain equations from a microscopic model of cardiac electrophysiology. Assuming an additional condition on the anisotropy, a simpler version is obtained and is called the monodomain model. Although it is less detailed than the bidomain model, the monodomain model is of great interest since it is much faster for simulation of the same problem compared to bidomain models. Moreover, for simulation of wave propagation in the heart, monodomain models reproduce many of the phenomena that are observed experimentally, and are thus a reliable tool [15, 30]. In a comparative study, Bourgault and Pierre [9] numerically estimated the discrepancy between the two models and they concluded that it is of order less than 1% in terms of activation time relative error noting that "this error is smaller than the discretisation error resulting from commonly used mesh size in biomedical engineering." Furthermore, for numerical simulations, they compared three methods for spatial discretization: the \mathbb{P}_1 finite element, the discrete duality finite volumes (DDFV), see for instance [3] as applied to the bidomain model) and control volumes finite elements (CVFE) and they concluded that the CVFE method gave the best results. The main purpose of this paper is to study a positive CVFE scheme for the monodomain model coupled to a physiologically based ionic model: the Beeler-Reuter model. We present in the following paragraphs a physiology and a modeling overview of the problem, then we give a summary of different related works.

The cardiac tissue is a complex structure composed mainly of elongated connected cells (cardiomyocytes) that have a cylindrical shape and that are aligned in preferential directions forming fibers. The contraction of these cells is initiated by an electrical signal (the action potential) and

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results in pumping blood to the whole body. Cardiomyocytes are encapsulated in a dynamic cell membrane (the sarcolemma) that separates the interior of the cell from the surrounding medium and maintains a potential difference (the transmembrane potential denoted by v) between the two media due to the varying concentrations of different ionic species on both sides of the membrane. The sarcolemma is a phospholipid bilayer in which are embedded ion channels. The latter are selectively permeable pores through which ions may flow under certain conditions. The ions of interest in cardiac electrophysiology are sodium Na⁺, potassium K⁺, and calcium Ca²⁺ [15, 29]. The movement of these ionic species across the membrane creates a current flow that changes the transmembrane potential. The currents associated to each ionic species are linearly added to give $I_{\rm ion}$ which represents the total current through the ion channels. In parallel, the membrane acts as a capacitor, so that the total current flow I_m through the membrane over time is given by

$$I_m = \chi \Big(C_m \frac{\partial v}{\partial t} + I_{\text{ion}}(v, \mathbf{w}) \Big),$$

where C_m is the membrane's capacitance by unit area, χ is the membrane surface area per unit volume and **w** is a state vector whose entries depend on the ionic model and represent the gating variables that model the openness of the ionic channels taken into consideration [29]. Furthermore, under the assumption of equal anisotropy ratios of the intra- and extracellular regions and using the Ohmic current-voltage relationship, the transmembrane current satisfies the relation

$$I_m = \nabla \cdot (\Lambda \nabla v),$$

where Λ is the conductivity tensor [29]. Equating the two entities above, the reaction diffusion equation of the monodomain model is obtained:

$$\chi C_m \frac{\partial v}{\partial t} - \nabla \cdot (\Lambda \nabla v) = -\chi I_{\text{ion}}(v, \mathbf{w}).$$

This equation is coupled through the vector \mathbf{w} to a system of ordinary differential equations representing the ionic model and given by:

$$\frac{\partial \mathbf{w}}{\partial t} = \mathbf{R}(v, \mathbf{w}).$$

The ionic model represented by this last equation and I_{ion} could be simple as in the FitzHugh-Nagumo model given by:

$$I_{\text{ion}} = c_1 v(v - \alpha)(1 - v) - c_2 w,$$

$$\frac{\partial w}{\partial t} = b(v - dw),$$

where c_1 and c_2 are the excitation rate and excitation decay constants respectively, α is the activation threshold value, and b and d are the recovery rate and recovery decay constants respectively [23]. In the present work, we investigate the monodomain model coupled to the Beeler-Reuter equations [5], which was one of the first mathematical models describing mammalian cardiac myocytes' electrophysiology. In fact, it is classified in the first-generation models which have been extensively used for studies of ventricular fibrillation, and which provide a good balance between numerical efficiency and biophysically important detail [15]. Although it may be considered simple compared to more recent models, it is able to realistically describe cell dynamics due to the presence of calcium concentration which is crucial for cardiac contraction.

From the numerical point of view, mathematical models for the propagation of electrical waves in the cardiac tissue have been extensively studied. We mention, for instance, the work of Harrild and Henriquez who gave a first approach in [26] and Trew et al. [31] who introduced a finite volume (FV) scheme for the bidomain equations representing physical discontinuities without the implicit removal of intracellular volume, giving rise to linear instead of nonlinear systems. Concerning the convergence analysis of FV schemes, a few works are available. Coudière and Pierre [16] proved convergence of an implicit FV approximation to the monodomain equations with FitzHugh-Nagumo ionic model. We mention also the work of Bendahmane and Karlsen [7] who analysed a FV method for the bidomain model with Dirichlet boundary conditions, supplying various existence, uniqueness and convergence results. We point out that in these works, the admissible mesh is adapted to the conductivity tensor and it is practically impossible to be constructed except under

isotropy condition. Moreover, Bendahmane, Bürger and Ruiz [6] analysed the bidomain equations formulated in a parabolic-elliptic form with Neumann boundary conditions, adapting the approach in [7], and providing some numerical experiments. We mention also the work of Andreianov et al. [3] who analyzed discrete duality finite volume (DDFV) approximations on distorted meshes for a class of simplified bidomain models (under a simplifying assumption on the ionic function). The latter discretization allowed to drop the restrictions on the mesh and on the isotropy of the conductivities. Practically, DDFV schemes fail to satisfy a discrete maximum principle [28] which is a crucial property when dealing with physical quantities such as the transmembrane potential, the gating and the concentration variables. These variables must verify some physiological bounds and this property is not guaranteed with DDFV discretization.

In the present work, we consider the monodomain model coupled to Beeler-Reuter cell model where physiological as well as mathematical considerations impose certain constraints on calcium concentration which appears as an argument of a logarithmic function and we need to guarantee its positivity. Moreover, the gating variables have to satisfy some physical bounds (between 0 and 1). We propose and analyze herein a nonlinear CVFE scheme obeying a maximum principle that may not be achieved for most finite element formulations but is crucial for our proof of convergence. Such schemes were proposed in [13] for solving degenerate anisotropic parabolic diffusion equations modeling flows in porous media and in [14] for a degenerate nonlinear chemotaxis model. We elaborate in the sequel an approach inspired from [13, 14] to approximate the non linear monodomain system over a general mesh with anisotropic conductivity tensor. In particular, a conforming piecewise linear finite element method on a primal triangular mesh is used along with the Godunov scheme to approximate the diffusion fluxes. This approach permits to obtain the discrete maximum principle without the assumption on the transmissibility coefficients to be positive. Indeed, this condition is very restrictive. It is verified for isotropic conductivities and for particular meshes. For instance, in case of a triangulation, the angles of the triangles must be acute. For more details about the analysis of the CVFE method for several partial differential equations we refer the reader to this non-exhaustive list [4, 12, 18, 21, 22].

This paper is organized as follows. First, the model, the mathematical assumptions and the weak formulation are presented in section 2. In section 3, the primal triangular mesh and the corresponding Donald dual mesh are defined. Then the discretization of the diffusion term is detailed to obtain the nonlinear CVFE scheme. The discrete maximum principle as well as several a priori estimates are established in section 4, leading to the existence of a discrete solution to the CVFE scheme. In section 5, compactness estimates are obtained on the approximate solutions leading to the passage along a subsequence to the limit which is shown to be a weak solution in section 6.

2. Mathematical Assumptions

We consider a bounded, open, polygonal, connected domain $\Omega \subset \mathbb{R}^d$, d=2, with boundary $\partial\Omega$, a fixed final time T>0, and we set $\Omega_T=(0,T)\times\Omega$.

Assuming an anisotropic medium, the conductivity is represented by the tensor $\Lambda(x)$ which is a bounded, uniformly positive symmetric tensor on Ω , that is, for all $\xi \in \mathbb{R}^d$:

$$\Lambda: \Omega \to \mathbb{R}^{d \times d}$$
, and $\exists m_0, M_0$ such that $0 < m_0 |\xi|^2 \le \Lambda \xi \cdot \xi \le M_0 |\xi|^2$, for a.e. $x \in \Omega$. (2.1)

Using Beeler-Reuter kinetics, the transmembrane potential $v:\Omega_T\to\mathbb{R}$ satisfies

$$\frac{\partial v}{\partial t} - \nabla \cdot (\Lambda(x)\nabla v) = -I_{\text{ion}}(v, m, o, l, f, r, z, [Ca^{++}]_i), \quad \text{for a.e. } (t, x) \in \Omega_T,$$
 (2.2)

where, for simplicity, we assumed that χ and C_m are equal to 1. The term $[Ca^{++}]_i: \Omega_T \to \mathbb{R}^+$ denotes the intracellular calcium concentration and the variables m, o, l, f, r, z are the components of the vector of gating variables $\mathbf{w}: \Omega_T \to \mathbb{R}^6$. Each of $w_j, j = 1, \dots, 6$ stands for m, o, l, f, r, z respectively, and obeys

$$\frac{\partial w_j}{\partial t} = \alpha_j(v)(1 - w_j) - \beta_j(v)w_j, \quad \text{for a.e. } (t, x) \in \Omega_T,$$
(2.3)

where α_j and β_j are Lipschitz continuous functions representing respectively the opening and closing rates and are given by [5, 29]

$$\alpha_j(v) = \frac{c_{1,j}e^{c_{2,j}(v+c_{3,j})} + c_{4,j}(v+c_{5,j})}{e^{c_{6,j}(v+c_{3,j})} + c_{7,j}},$$

and

$$\beta_j(v) = \frac{d_{1,j}e^{d_{2,j}(v+d_{3,j})} + d_{4,j}(v+d_{5,j})}{e^{d_{6,j}(v+d_{3,j})} + d_{7,j}},$$

for given constants $d_{i,j}$, $c_{i,j}$, $i = 1, \dots, 7$, $j = 1, \dots, 6$ such that

$$\alpha_j(v), \beta_j(v) > 0. \tag{2.4}$$

The function $I_{\text{ion}}: \mathbb{R} \times \mathbb{R}^6 \times \mathbb{R}^+ \to \mathbb{R}$ is the collection of membrane currents, and the charge flow through the membrane is assumed to include four individual currents [5, 29]. The direction of two of these, representing the flow of potassium (K^+) ions, points out of the cell:

$$I_{Pot}(v) = 1.4 \frac{e^{0.04(v+85)} - 1}{e^{0.08(v+53)} + e^{0.04(v+53)}} + 0.07 \frac{v+23}{1 - e^{-0.04(v+23)}},$$
(2.5)

and

$$I_z(v,z) = 0.8z \frac{e^{0.04(v+77)} - 1}{e^{0.04(v+35)}}. (2.6)$$

There are also two inward currents; the first is the inward current of sodium (Na^+) ions:

$$I_{Na}(v, m, o, l) = (g_{Na}m^{3}ol + g_{Na}C)(v - E_{Na}),$$
(2.7)

where $E_{Na} = 50$ is the equilibrium potential of sodium, $g_{Na} = 4$ is the membrane conductivity of the sodium current and $g_{NaC} = 0.003$ is the membrane conductivity of the sodium-calcium exchanger current [5]. The second inward current is the slow inward current given by:

$$I_s(v, f, r, \lceil Ca^{++} \rceil_i) = g_s fr(v + 82.3 + 13.0287 \ln(\lceil Ca^{++} \rceil_i)). \tag{2.8}$$

The latter is carried primarily but not exclusively by calcium ions across the membrane and $g_s = 0.09$ is the conductivity related to the slow inward current. As a result, the total ionic current is given by:

$$I_{\text{ion}}(v, \mathbf{w}, [Ca^{++}]_i) = I_{Pot}(v) + I_z(v, z) + I_{Na}(v, m, o, l) + I_s(v, f, r, [Ca^{++}]_i).$$

The intracellular calcium concentration $[Ca^{++}]_i$ is scaled like $c = 10^3 [Ca^{++}]_i$ and fulfills the ODE [25]

$$\frac{\partial c}{\partial t} = 0.07(10^{-4} - c) - 10^{-4} I_s(v, f, r, c), \quad \text{for a.e. } (t, x) \in \Omega_T,$$
(2.9)

where

$$I_s(v, f, r, c) = g_s fr(v - 7.7 + 13.0287 \ln(c)).$$

We refer to (2.2), (2.3), (2.9) as the equations of the monodomain model with Beeler-Reuter kinetics together with Neumann boundary condition imposed on v:

$$\Lambda(x)\nabla v \cdot \mathbf{n} = 0 \text{ for a.e. } (t, x) \in (0, T) \times \partial\Omega,$$
 (2.10)

where \mathbf{n} is the outward unit normal, and with the initial Cauchy conditions:

$$v(0,x) = v_0(x), \quad \mathbf{w}(0,x) = \mathbf{w}_0(x), \quad c(0,x) = c_0(x) \text{ for a.e. } x \in \Omega.$$

The initial data $(v_0, \mathbf{w}_0, c_0) \in (L^{\infty}(\Omega), (H^1(\Omega))^6, H^1(\Omega))$, are assumed to satisfy

$$v_m \le v_0 \le v_M$$
 a.e. in Ω ,
 $c_m \le c_0 \le c_M$ a.e. in Ω ,
 $0 \le w_{0,j} \le 1$ a.e. in Ω , for $j = 1, \dots, 6$ (2.11)

where $v_m = -85$, $v_M = 127.69$, $c_m = 10^{-4}$ and $c_M = 0.0187$ are given constants such that $I_s(v_M, f, r, c_m) = 0$. We refer to [25] for a heuristic motivation of these values and to ([5],[29]) for a complete description of the model.

For simplicity of the calculations herein, we introduce a rescaling \tilde{v} of the potential difference v given by the relation:

$$\tilde{v} = \frac{v - v_m}{v_M - v_m},$$

and we denote by

$$\tilde{I}_{\text{ion}}(\tilde{v}, \mathbf{w}, c) := \frac{1}{v_M - v_m} I_{\text{ion}}((v_M - v_m)\tilde{v} + v_m, \mathbf{w}, c),$$

$$\tilde{\alpha}_j(\tilde{v}) := \alpha_j((v_M - v_m)\tilde{v} + v_m),$$

$$\tilde{\beta}_j(\tilde{v}) := \beta_j((v_M - v_m)\tilde{v} + v_m),$$

and

$$\tilde{I}_{s,1}(\tilde{v}, f, r, c) := I_s((v_M - v_m)\tilde{v} + v_m, f, r, c).$$

So assumption (2.11) becomes:

$$0 \le \tilde{v}_0 \le 1 \quad \text{in } \Omega,$$

$$c_m \le c_0 \le c_M \quad \text{in } \Omega,$$

$$0 \le w_{0,j} \le 1 \quad \text{in } \Omega, \text{ for } j = 1, \dots, 6.$$

$$(2.12)$$

We further notice that the ionic function \tilde{I}_{ion} verifies for all $w_j \in [0,1], j=1,\cdots,6$ and $c \in [c_m,c_M]$

$$\tilde{I}_{\text{ion}}(0, \mathbf{w}, c) \le 0 \text{ and } \tilde{I}_{\text{ion}}(1, \mathbf{w}, c) \ge 0.$$
 (2.13)

To summarize, we have the following system of equations:

$$\begin{split} \frac{\partial \tilde{v}}{\partial t} &= \nabla \cdot (\Lambda \nabla \tilde{v}) - \tilde{I}_{\text{ion}}(\tilde{v}, \mathbf{w}, c), & \text{for a.e. } (t, x) \in \Omega_T, \\ \frac{\partial w_j}{\partial t} &= \tilde{\alpha}_j(\tilde{v})(1 - w_j) - \tilde{\beta}_j(\tilde{v})w_j, & \text{for a.e. } (t, x) \in \Omega_T \text{ and } j = 1, \cdots, 6, \\ \frac{\partial c}{\partial t} &= 0.07(10^{-4} - c) - 10^{-4}\tilde{I}_{s,1}(\tilde{v}, f, r, c), & \text{for a.e. } (t, x) \in \Omega_T, \\ \tilde{v}(0, x) &= \tilde{v}_0(x), & \text{for a.e. } x \in \Omega, \\ \mathbf{w}(0, x) &= \mathbf{w}_0(x), & \text{for a.e. } x \in \Omega, \\ c(0, x) &= c_0(x), & \text{for a.e. } x \in \Omega \\ \Lambda \nabla \tilde{v} \cdot \mathbf{n} &= 0 & \text{a.e. on } \partial \Omega \times (0, T). \end{split}$$

For simplicity of notation, we will omit in what follows the \sim symbol.

2.1. **Weak Formulation.** Before defining the discrete scheme, we provide a relevant definition of a weak solution for the monodomain model.

Definition 2.1. A weak solution of (2.14) is a vector $\mathbf{U} = (v, \mathbf{w}, c)$, of functions such that $v \in L^{\infty}(\Omega_T) \cap L^2(0, T; H^1(\Omega))$, $\mathbf{w} \in \left(L^{\infty}(\Omega_T)\right)^6$, $c \in L^{\infty}(\Omega_T)$, with $0 \le v \le 1$, $0 \le w_j \le 1$ for $j = 1, \dots, 6$, $0 < c_m \le c \le c_M$, and for all φ , ψ and $\xi \in D([0, T) \times \overline{\Omega})$, there holds:

$$-\int_{\Omega} v_0(x)\varphi(0,x)dx + \iint_{\Omega_T} \left(-v\partial_t \varphi + \Lambda \nabla v \cdot \nabla \varphi\right) dxdt = \iint_{\Omega_T} -I_{\text{ion}}(v,\mathbf{w},c)\varphi dxdt, \quad (2.15)$$

$$-\int_{\Omega} w_{0,j}(x)\psi(0,x)dx + \iint_{\Omega_T} -w_j\partial_t\psi dxdt = \iint_{\Omega_T} (\alpha_j(v)(1-w_j) - \beta_j(v)w_j)\psi dxdt, \quad (2.16)$$

for $j = 1, \dots, 6$, and

$$-\int_{\Omega} c_0(x)\xi(0,x)dx + \iint_{\Omega_T} -c\partial_t \xi dxdt = \iint_{\Omega_T} (0.07(10^{-4} - c) - 10^{-4}I_{s,1}(v,f,r,c))\xi dxdt.$$
 (2.17)

Remark 2.1. Observe that in Definition 2.1, we do not need the time continuity of v. In general, in the case of numerical schemes, there are no compactness results that allow to prove the time continuity of the solutions. However, one can make use of the weak formulation to prove that the limit solution v is continuous in time (see for instance [10]).

3. Discrete Problem

3.1. **Space Discretization.** Following [13, 14], we give a precise definition of the CVFE scheme for the monodomain equations.

We recall that Ω is an open, bounded, connected polygonal domain in \mathbb{R}^d , d=2, with boundary $\partial\Omega$. Let \mathcal{T} be a conforming triangulation of Ω . We assume that $\bigcup_{T\in\mathcal{T}}\bar{T}=\bar{\Omega}$. We denote by \mathcal{V} the set of vertices (located at positions $(x_K)_{K\in\mathcal{V}}$) and by \mathcal{E} the set of edges of the triangulation \mathcal{T} . For $T\in\mathcal{T}$, \mathcal{E}_T denotes the subset of edges σ such that $\bigcup_{\sigma\in\mathcal{E}_T}\sigma=\partial T$. We also assume that $\mathcal{E}=\bigcup_{T\in\mathcal{T}}\mathcal{E}_T$.

For $T \in \mathcal{T}$, x_T denotes the center of gravity of T, h_T the diameter of the triangle T, and ρ_T the diameter of the circle inscribed in T. Then we define the mesh diameter h and the mesh regularity θ_T by

$$h = \max_{T \in \mathcal{T}} h_T, \qquad \quad \theta_{\mathcal{T}} = \max_{T \in \mathcal{T}} \frac{h_T}{\rho_T}.$$

For $K \in \mathcal{V}$, the subset of \mathcal{T} made of triangles that have K as a vertex are denoted by \mathcal{T}_K , and the set of edges having the vertex K at an extremity by \mathcal{E}_K . Furthermore, the subset \mathcal{V}_K of \mathcal{V} consists of vertices L that share a common edge with K.

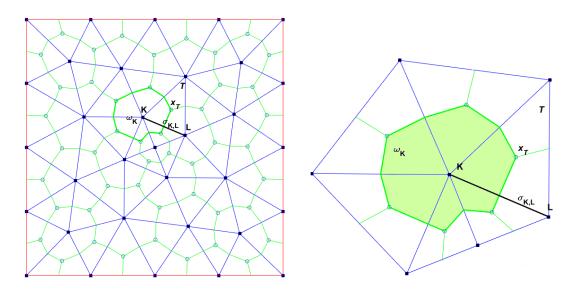


FIGURE 1. Triangular mesh \mathcal{T} (in blue), dual mesh \mathcal{M} (in green)

Once the primal triangular discretization is constructed, we build a different space discretization of Ω called the dual barycentric discretization \mathcal{M} . To each $K \in \mathcal{V}$, we associate a control volume ω_K (of measure m_K) which vertices are the centers of gravity x_T of the triangles $T \in \mathcal{T}_K$ and the barycenters of the edges $\sigma \in \mathcal{E}_K$. We note that $\bar{\Omega} = \bigcup_{K \in \mathcal{V}} \bar{\omega}_K$.

3.2. **Discrete Spaces.** We construct two discrete functional spaces corresponding to the primal and dual meshes. The first one is the usual \mathbb{P}_1 -conforming finite element space denoted by:

$$V_{\mathcal{T}} = \{ f \in C(\Omega); f|_T \in \mathbb{P}_1(\mathbb{R}^d), \forall T \in \mathcal{T} \}.$$

We also define the space $X_{\mathcal{M}}$ of piecewise constant functions on the dual cells by

$$X_{\mathcal{M}} = \{ f: \Omega \to \bar{\mathbb{R}} \text{ measurable}; f|_{\omega_K} \in \mathbb{P}_0(\mathbb{R}^d), \forall K \in \mathcal{V} \}.$$

Given a vector $(v_K)_{K \in \mathcal{V}} \in \mathbb{R}^{\operatorname{Card}(\mathcal{V})}$, there exists a unique $v_{\mathcal{T}} \in V_{\mathcal{T}}$ and a unique $v_{\mathcal{M}} \in X_{\mathcal{M}}$ such that

$$v_{\mathcal{T}}(x_K) = v_{\mathcal{M}}(x_K) = v_K, \quad \forall K \in \mathcal{V}.$$

In what follows, we denote by $(e_K)_{K\in\mathcal{V}}$ the canonical basis of $V_{\mathcal{T}}$, characterized by

$$e_K(x_L) = \delta_{KL}, \quad \forall K \in \mathcal{V}.$$

We remark that

$$\sum_{K \in \mathcal{V}} e_K(x) = 1, \qquad \forall x \in \Omega.$$

Therefore

$$\sum_{K\in\mathcal{V}}\int_{\Omega}e_K(x)dx=|\Omega|,$$

and

$$\sum_{K \in \mathcal{V}} \nabla e_K(x) = 0, \text{ for a.e.} x \in \Omega.$$
(3.1)

We use the finite element approximations for $v, w_j, j = 1, \dots, 6$ and c, where:

$$v \approx v_{\mathcal{T}} = \sum_{L \in \mathcal{V}} v_L e_L, \quad w_j \approx w_{j,\mathcal{T}} = \sum_{L \in \mathcal{V}} w_{j,L} e_L, \text{ and } c \approx c_{\mathcal{T}} = \sum_{L \in \mathcal{V}} c_L e_L.$$

For all $(K, L) \in \mathcal{V}^2$, we define the transmissibility coefficient Λ_{KL} by

$$\Lambda_{KL} = -\int_{\Omega} \Lambda(x) \nabla e_K(x) \cdot \nabla e_L(x) dx = \Lambda_{LK}. \tag{3.2}$$

Due to (3.1), we have $\Lambda_{KK} = -\sum_{L \neq K} \Lambda_{KL} < 0$. As a result, we have

$$\int_{\Omega} \Lambda(x) \nabla v_{\mathcal{T}} \cdot \nabla \varphi_{\mathcal{T}} = \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} (v_K - v_L) (\varphi_K - \varphi_L). \tag{3.3}$$

- 3.3. **Time Discretization.** The discretization of the time interval (0,T) is given by a time step Δt , and a positive integer N chosen such that $N\Delta t = T$. We set $t_n = n\Delta t$ for $n \in \{0, ..., N\}$.
- 3.4. **Space-time Discretization.** We define the space and time discrete spaces $V_{\mathcal{T},\Delta t}$ and $X_{\mathcal{M},\Delta t}$ as the set of piecewise constant functions in time with values in $V_{\mathcal{T}}$ and $X_{\mathcal{M}}$ respectively, i.e.:

$$f \in V_{\mathcal{T},\Delta t} \Leftrightarrow f(t,x) = f(t_{n+1},x) \in V_{\mathcal{T}}, \ \forall t \in (t_n,t_{n+1}],$$

and

$$f \in X_{\mathcal{M},\Delta t} \Leftrightarrow f(t,x) = f(t_{n+1},x) \in X_{\mathcal{M}}, \ \forall t \in (t_n,t_{n+1}].$$

For a given $(v_K^{n+1})_{n\in\{0,\dots,N-1\},K\in\mathcal{V}}\in\mathbb{R}^{N\mathrm{Card}(\mathcal{V})}$, we denote the unique elements $v_{\mathcal{T},\Delta t}\in V_{\mathcal{T},\Delta t}$ and $v_{\mathcal{M},\Delta t}\in X_{\mathcal{M},\Delta t}$ such that

$$v_{\mathcal{T},\Delta t}(t, x_K) = v_{\mathcal{M},\Delta t}(t, x_K) = v_K^{n+1}, \quad \forall K \in \mathcal{V}, \forall t \in (t_n, t_{n+1}].$$

3.5. The CVFE Scheme. In order to discretize the equations of (2.14), we formally integrate the equations over $(t_n, t_{n+1}) \times \omega_K$ and we use Green's theorem on the diffusive term; we obtain:

$$\int_{\omega_{K}} v(t_{n+1}, x) - v(t_{n}, x) dx = \int_{t_{n}}^{t_{n+1}} \int_{\partial \omega_{K}} (\Lambda \nabla v) \cdot \mathbf{n} d\gamma dt - \int_{t_{n}}^{t_{n+1}} \int_{\omega_{K}} I_{ion}(v, m, o, l, f, r, z, c) dx dt,$$

$$\int_{\omega_{K}} w_{j}(t_{n+1}, x) - w_{j}(t_{n}, x) dx = \int_{t_{n}}^{t_{n+1}} \int_{\omega_{K}} (\alpha_{j}(v)(1 - w_{j}) - \beta_{j}(v)w_{j}) dx dt, \text{ for } j = 1, \dots, 6,$$

$$\int_{\omega_{K}} c(t_{n+1}, x) - c(t_{n}, x) dx = \int_{t_{n}}^{t_{n+1}} \int_{\omega_{K}} (0.07(10^{-4} - c) - 10^{-4}I_{s,1}(v, f, r, c)) dx dt.$$

We use a time discretization in which the linear terms of the ODEs correspoding to the recovery variables are implicitly discretized whereas the nonlinear terms are considered explicitly. In order to ensure the maximum principle, the potential difference v in the ionic function and the logarithmic term of the ODE involving the concentration variable c are considered implicitly. We propose the following semi-implicit CVFE scheme:

We look for $(v_K^{n+1})_{K\in\mathcal{V},n\in\{0,\cdots,N-1\}}$, $(\mathbf{w}_K^{n+1})_{K\in\mathcal{V},n\in\{0,\cdots,N-1\}}$, and $(c_K^{n+1})_{K\in\mathcal{V},n\in\{0,\cdots,N-1\}}$ solution of the nonlinear system: $\forall K\in\mathcal{V}$,

$$v_K^0 = \frac{1}{m_K} \int_{\omega_K} v_0(x) dx, \mathbf{w}_K^0 = \frac{1}{m_K} \int_{\omega_K} \mathbf{w}_0(x) dx, \text{ and } c_K^0 = \frac{1}{m_K} \int_{\omega_K} c_0(x) dx$$
 (3.4)

and $\forall n \in \{0, \dots, N-1\}, \forall K \in \mathcal{V},$

$$\frac{m_K}{\Delta t}(v_K^{n+1} - v_K^n) + \sum_{\sigma_{KL} \in \mathcal{E}_K} \Lambda_{KL}(v_K^{n+1} - v_L^{n+1})
= -m_K \Big(I_{Pot}(v_K^{n+1}) + I_z(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_{Na}(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_s(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \Big),$$
(3.5)

$$w_{j,K}^{n+1} - w_{j,K}^{n} = \Delta t \left(\alpha_j(v_K^n) (1 - w_{j,K}^{n+1}) - \beta_j(v_K^n) w_{j,K}^{n+1} \right), \text{ for } j = 1, \dots, 6,$$
(3.6)

$$c_K^{n+1} - c_K^n = \Delta t \Big(0.07(10^{-4} - c_K^{n+1}) - g_s 10^{-4} f_K^{n+1} r_K^{n+1} (v_K^{n+1} - 7.7 + 13.0287 \ln(c_K^{n+1})) \Big), \quad (3.7)$$

where the transmissibility coefficient Λ_{KL} is defined by (3.2). However, for general triangulations and/or for anisotropic tensors Λ , this discretization does not guarantee the monotonicity of the discrete diffusion operator and hence the obtention of the discrete maximum principle [13]. For this reason, we introduce the functions $\eta(v)$, p(v), $\Gamma(v)$ and $\phi(v)$ defined by:

$$\eta(v) = \begin{cases}
v(1-v), & \text{if } 0 \le v \le 1, \\
0, & \text{if } v \le 0 \text{ or } v > 1,
\end{cases}$$
(3.8)

$$p(v) = \ln\left(\frac{v}{1-v}\right), \text{ if } 0 < v < 1, \tag{3.9}$$

$$\Gamma(v) = v \ln(v) + (1 - v) \ln(1 - v), \text{ if } 0 < v < 1,$$
 (3.10)

$$\phi(v) = 2\arcsin\sqrt{v}, \text{ if } 0 \le v \le 1. \tag{3.11}$$

We use herein the convention

$$\eta(v)p(v) = 0$$
 $v < 0$ and $v > 1$.

Note that, by the mean value theorem, there holds

$$\frac{p(x) - p(y)}{x - y} = p'(b) = \frac{1}{\eta(b)}, \text{ for some } b \in (x, y)$$

and then

$$x - y = \eta(b)(p(x) - p(y)).$$

The discrete equation (3.5) is now replaced by

$$\frac{m_K}{\Delta t} (v_K^{n+1} - v_K^n) + \sum_{\sigma_{KL} \in \mathcal{E}_K} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))
= -m_K \Big(I_{Pot}(v_K^{n+1}) + I_z(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_{Na}(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_s(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \Big)$$
(3.12)

where, denoting by

$$J_{KL}^{n+1} = [\min(v_K^{n+1}, v_L^{n+1}), \max(v_K^{n+1}, v_L^{n+1})], \tag{3.13}$$

we have set

$$\eta_{KL}^{n+1} = \begin{cases} \max_{s \in J_{KL}^{n+1}} \eta(s) & \text{if } \Lambda_{KL} \ge 0, \\ \min_{s \in J_{KL}^{n+1}} \eta(s) & \text{if } \Lambda_{KL} < 0. \end{cases}$$
(3.14)

Remark 3.1. Note that due to the use of the function p in the scheme, (3.12) does not make sense unless

$$0 < v_K^{n+1} < 1 \qquad \forall \ K \in \mathcal{V}, \ \forall \ n \ge 0.$$

This will be assumed in the a priori estimates and proved later in Lemma 4.10 and Lemma 4.11.

3.6. Main result. Let $(\mathcal{T}_m)_{m\geq 1}$ be a sequence of triangulations of Ω such that

$$h_m = \max_{T \in \mathcal{T}_m} \operatorname{diam}(T) \to 0 \text{ as } m \to \infty,$$

and assume that the sequence of triangulations has a bounded regularity, in other words, there exists a constant $\theta > 0$ such that

$$\theta_{\mathcal{T}_m} \leq \theta, \ \forall \ m \geq 1.$$

A sequence of barycentric dual meshes $(\mathcal{M}_m)_{m\geq 1}$ is also constructed. Furthermore, for an increasing sequence of integers $(N_m)_{m\geq 1}$, define the corresponding sequence of time steps $(\Delta t_m)_{m\geq 1}$ such that $\Delta t_m \to 0$ as $m \to \infty$. The main purpose of this work is to prove the following theorem.

Theorem 3.1. There exists a sequence $(v_{\mathcal{M}_m,\Delta t_m}, \mathbf{w}_{\mathcal{M}_m,\Delta t_m}, c_{\mathcal{M}_m,\Delta t_m})_m$ of solutions to the scheme (3.12),(3.6),(3.7), such that $0 \leq v_{\mathcal{M}_m,\Delta t_m} \leq 1$, $0 \leq w_{j,\mathcal{M}_m,\Delta t_m} \leq 1$ for $j = 1, \dots, 6$, $c_m \leq c_{\mathcal{M}_m,\Delta t_m} \leq c_M$ and

$$v_{\mathcal{M}_m,\Delta t_m} \to v$$
, $\mathbf{w}_{\mathcal{M}_m,\Delta t_m} \to \mathbf{w}$, and $c_{\mathcal{M}_m,\Delta t_m} \to c$ a.e. in Ω_T as $m \to \infty$,

where the triplet (v, \mathbf{w}, c) is a weak solution to System (2.14) as in Definition 2.1.

The rest of the paper is devoted to the proof of the above theorem which is organized as follows: in section 4, some discrete properties, the discrete maximum principle, some a priori estimates and the existence of the discrete solution are obtained. The compactness estimates and the passage to the limit are established in section 5. Finally, the identification of the limit functions as a weak solution is proved in section 6. Furthermore, in the last section of the paper, some numerical tests are shown.

4. Discrete properties, a priori estimates and existence of a discrete solution

4.1. Discrete Maximum Principle.

Lemma 4.1. Let $(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^{n+1})_{K \in \mathcal{V}, n \in \{0, \dots, N-1\}}$ be a solution of the CVFE scheme (3.12), (3.6), (3.7). Then for all $K \in \mathcal{V}$, and $n \in \{0, \dots, N-1\}$, we have: $0 \le w_{j,K}^{n+1} \le 1$, $j = 1, \dots, 6$, $c_m \le c_K^{n+1} \le c_M$ and $0 \le v_K^{n+1} \le 1$.

Proof. We use induction over n. Due to assumption (2.11), the assertion is true for n = 0. We assume it true for n, and we prove it true for n + 1.

In the following, the index j is skipped in order to simplify the notation. Define

$$\chi(x) = \left\{ \begin{array}{ll} 1-x & \text{if } x \leq 1, \\ 0 & \text{if } x > 1, \end{array} \right.$$

and write equation (3.6) as: for all $K \in \mathcal{V}$,

$$w_K^{n+1} - w_K^n = \Delta t \Big(\alpha(v_K^n) \chi(w_K^{n+1}) - \beta(v_K^n) w_K^{n+1} \Big). \tag{4.1}$$

Multiplying first (4.1) by $-(w_K^{n+1})^- := \min(w_K^{n+1}, 0)$, one obtains:

$$\begin{split} |(w_K^{n+1})^-|^2 &= -w_K^n (w_K^{n+1})^- + \Big[-\alpha(v_K^n) \chi(w_K^{n+1}) (w_K^{n+1})^- + \beta(v_K^n) w_K^{n+1} (w_K^{n+1})^- \Big] \Delta t \\ &= -w_K^n (w_K^{n+1})^- + \Big[-\alpha(v_K^n) \chi(w_K^{n+1}) (w_K^{n+1})^- - \beta(v_K^n) \Big((w_K^{n+1})^- \Big)^2 \Big] \Delta t \\ &< 0. \end{split}$$

The last inequality implies that $(w_K^{n+1})^- = 0$ and $w_K^{n+1} \ge 0$. Therefore, $w_K^{n+1} \ge 0$ for all $K \in \mathcal{V}$. Using the same reasoning, multiply equation (4.1) by $(w_K^{n+1} - 1)^+ := max(0, w_K^{n+1} - 1)$ to obtain

$$|(w_K^{n+1}-1)^+|^2 = (w_K^n-1)(w_K^{n+1}-1)^+ + \left[\alpha(v_K^n)\chi(w_K^{n+1})(w_K^{n+1}-1)^+ - \beta(v_K^n)w_K^{n+1}(w_K^{n+1}-1)^+\right]\Delta t.$$

By definition of the function χ , one can easily check that $\chi(w_K^{n+1})(w_K^{n+1}-1)^+ \leq 0$. Moreover, exploiting the positivity of w_K^{n+1} , one has $w_K^{n+1}(w_K^{n+1}-1)^+ \geq 0$ and making use of the inductive hypothesis, one also has $w_K^n - 1 \leq 0$. As a result, there holds $|(w_K^{n+1}-1)^+|^2 \leq 0$. Therefore, $w_K^{n+1} \leq 1$ for all $K \in \mathcal{V}$.

In order to prove that $0 \le v_K^{n+1} \le 1$, consider a fixed dual control volume ω_K such that $v_K^{n+1} = \min_{L \in \mathcal{V}} (v_L^{n+1})$ and assume that $v_K^{n+1} < 0$ trying to obtain a contradiction.

Multiplying equation (3.12) by $-(v_K^{n+1})^-$, we obtain

$$m_{K} \left| (v_{K}^{n+1})^{-} \right|^{2} = -m_{K} v_{K}^{n} (v_{K}^{n+1})^{-} + \Delta t \sum_{\sigma \in \mathcal{E}_{K}} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_{K}^{n+1}) - p(v_{L}^{n+1})) (v_{K}^{n+1})^{-}$$

$$+ m_{K} \Delta t \left(I_{Pot}(v_{K}^{n+1}) + I_{z}(v_{K}^{n+1}, z_{K}^{n+1}) + I_{Na}(v_{K}^{n+1}, m_{K}^{n+1}, o_{K}^{n+1}, l_{K}^{n+1}) \right)$$

$$+ I_{s}(v_{K}^{n+1}, f_{K}^{n+1}, r_{K}^{n+1}, c_{K}^{n}) (v_{K}^{n+1})^{-}$$

In view of the definition of η_{KL}^{n+1} given in (3.14), and of the fact that $\eta(v) = 0$ if $v \leq 0$, we have $\eta_{KL}^{n+1} = 0$ if $\Lambda_{KL} \leq 0$. Therefore, the second term on the left hand side of the above equation is reduced to:

$$\Delta t \sum_{\sigma \in \mathcal{E}_K} (\Lambda_{KL})^+ \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1})) (v_K^{n+1})^-,$$

and by monotonicity of p, we have

$$p(v_K^{n+1}) - p(v_L^{n+1}) \le 0.$$

Thus, we get

$$m_{K} \left| (v_{K}^{n+1})^{-} \right|^{2} \leq m_{K} \Delta t \left(I_{Pot}(v_{K}^{n+1}) + I_{z}(v_{K}^{n+1}, z_{K}^{n+1}) + I_{Na}(v_{K}^{n+1}, m_{K}^{n+1}, o_{K}^{n+1}, l_{K}^{n+1}) + I_{s}(v_{K}^{n+1}, f_{K}^{n+1}, r_{K}^{n+1}, c_{K}^{n}) \right) (v_{K}^{n+1})^{-}.$$

$$(4.2)$$

Let us show that

$$m_K \left| (v_K^{n+1})^- \right|^2 \le 0.$$

Recalling that the expressions of I_{Pot} and I_z (after rescaling v) are given by:

$$I_{Pot}(v) = \frac{1}{v_M - v_m} \left(1.4 \frac{e^{0.04((v_M - v_m)v)} - 1}{e^{0.08((v_M - v_m)v - 32)} + e^{0.04((v_M - v_m)v - 32)}} + 0.07 \frac{(v_M - v_m)v - 62}{1 - e^{-0.04((v_M - v_m)v - 62)}} \right)$$

and

$$I_z(v,z) = \frac{1}{v_M - v_m} \left(0.8z \frac{e^{0.04((v_M - v_m)v - 8)} - 1}{e^{0.04((v_M - v_m)v - 50)}} \right),$$

one can easily verify that if $v_K^{n+1} < 0$, then $I_{Pot} \le 0$ and $I_z \le 0$. Moreover, the third term on the right hand side of (4.2) can be rearranged as follows

$$\begin{split} &I_{Na}(v_K^{n+1},m_K^{n+1},o_K^{n+1},l_K^{n+1})\Big(v_K^{n+1}\Big)^-\\ &= \frac{1}{v_M-v_m}[(g_{Na}(m_K^{n+1})^3o_K^{n+1}l_K^{n+1}+g_{NaC})((v_M-v_m)v_K^{n+1}+v_m-E_{Na})(v_K^{n+1})^-]\\ &= -(g_{Na}(m_K^{n+1})^3o_K^{n+1}l_K^{n+1}+g_{NaC})|(v_K^{n+1})^-|^2\\ &\quad + \frac{1}{v_M-v_m}(g_{Na}(m_K^{n+1})^3o_K^{n+1}l_K^{n+1}+g_{NaC})(v_m-E_{Na})(v_K^{n+1})^-\\ &\leq 0. \end{split}$$

Also, one can write $I_s(v_K^{n+1},f_K^{n+1},r_K^{n+1},c_K^n)(v_K^{n+1})^-$ as

$$\begin{split} I_{s}(v_{K}^{n+1},f_{K}^{n+1},r_{K}^{n+1},c_{K}^{n})(v_{K}^{n+1})^{-} &= \frac{1}{v_{M}-v_{m}}g_{s}f_{K}^{n+1}r_{K}^{n+1}((v_{M}-v_{m})v_{K}^{n+1} \\ &+v_{m}-7.7+13.028\ln(c_{K}^{n}))(v_{K}^{n+1})^{-} \\ &= -g_{s}f_{K}^{n+1}r_{K}^{n+1}\left|(v_{K}^{n+1})^{-}\right|^{2} \\ &+ \frac{1}{v_{M}-v_{m}}g_{s}f_{K}^{n+1}r_{K}^{n+1}(v_{m}-7.7+13.028\ln(c_{K}^{n}))(v_{K}^{n+1})^{-} \\ &\leq 0, \end{split}$$

where the last inequality is a consequence of the hypothesis $c_m \leq c_K^n \leq c_M$ and the positivity of f_K^{n+1} and r_K^{n+1} . We conclude therefore that $(v_K^{n+1})^- = 0$ which contradicts the assumption that $v_K^{n+1} < 0$. Hence, $v_K^{n+1} \geq 0$. Similarly, one can prove that $v_K^{n+1} \leq 1$, by using (3.12) over the dual control volume ω_K such that: $v_K^{n+1} = \max_{L \in \mathcal{V}} (v_L^{n+1})$, then multiplying equation (3.12) by $(v_K^{n+1} - 1)^+$.

Now, we show that $c_m \leq c_K^{n+1} \leq c_M$. Define, first, the function

$$F(v, f, r, c) = 0.07(10^{-4} - c) - 10^{-4}I_s(v, f, r, c).$$

Then assume that $c_K^{n+1} < c_m$ and multiply (3.7) by $-(c_K^{n+1} - c_m)^- := \min(0, c_K^{n+1} - c_m)$, to get:

$$-c_K^{n+1}(c_K^{n+1}-c_m)^- = -c_K^n(c_K^{n+1}-c_m)^- - \Delta t F(v_K^{n+1},f_K^{n+1},r_K^{n+1},c_K^{n+1})(c_K^{n+1}-c_m)^-,$$

or equivalently

$$[(c_K^{n+1} - c_m)^-]^2 = -(c_K^n - c_m)(c_K^{n+1} - c_m)^- - \Delta t F(v_K^{n+1}, f_K^{n+1}, r_K^{n+1}, c_K^{n+1})(c_K^{n+1} - c_m)^-.$$

Since $c_K^n \ge c_m$, then

$$\begin{split} [(c_K^{n+1}-c_m)^-]^2 & \leq & -\Delta t F(v_K^{n+1},f_K^{n+1},r_K^{n+1},c_K^{n+1})(c_K^{n+1}-c_m)^- \\ & = & -\Delta t [F(v_K^{n+1},f_K^{n+1},r_K^{n+1},c_K^{n+1}) - F(v_K^{n+1},f_K^{n+1},r_K^{n+1},c_m)](c_K^{n+1}-c_m)^- \\ & & -\Delta t F(v_K^{n+1},f_K^{n+1},r_K^{n+1},c_m)(c_K^{n+1}-c_m)^-, \end{split}$$

Noting that $\frac{\partial F}{\partial c} < 0$, one has

$$F(v_K^{n+1}, f_K^{n+1}, r_K^{n+1}, c_K^{n+1}) - F(v_K^{n+1}, f_K^{n+1}, r_K^{n+1}, c_m) \ge 0.$$

Consequently, one gets

$$[(c_K^{n+1} - c_m)^-]^2 \le -\Delta t F(v_K^{n+1}, f_K^{n+1}, r_K^{n+1}, c_m)(c_K^{n+1} - c_m)^-$$

$$\le 0,$$

where the last inequality follows since $F(v_K^{n+1}, f_K^{n+1}, r_K^{n+1}, c_m) \ge 0$ for $0 \le v_K^{n+1} \le 1$. So $(c_K^{n+1} - c_m)^- = 0$ and $c_K^{n+1} \ge c_m$ which contradicts the assumption that $c_K^{n+1} < c_m$. Hence $c_K^{n+1} \ge c_m$. We repeat the argument by multiplying (3.7) by $(c_K^{n+1} - c_M)^+ := \max(0, c_K^{n+1} - c_M)$ to obtain $c_K^{n+1} \le c_M$.

4.2. Discrete Properties.

Lemma 4.2. Let $(v_K^{n+1})_{K,n} \in \mathbb{R}^{NCard(\mathcal{V})}$, then denoting by $\phi_{\mathcal{T},\Delta t}$ the unique function in $V_{\mathcal{T},\Delta t}$ with nodal values $\phi(v_K^{n+1})$ (ϕ defined in (3.11)), there holds

$$\sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2$$
(4.3)

$$\geq \sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} (\phi(v_K^{n+1}) - \phi(v_L^{n+1}))^2 = \iint_{\Omega_T} \Lambda \nabla \phi_{\mathcal{T}, \Delta t} \cdot \nabla \phi_{\mathcal{T}, \Delta t} dx dt$$

Proof. This result can be found in [13], we reproduce the proof herein for the sake of completeness. We first note that by Cauchy's mean value theorem, we have:

$$\frac{\phi(v_K^{n+1}) - \phi(v_L^{n+1})}{p(v_K^{n+1}) - p(v_I^{n+1})} = \sqrt{\eta(b)}, \text{ for some } b \in J_{KL}^{n+1},$$

since for $x \in (0,1)$, $\phi' = \frac{1}{\sqrt{\eta}}$, $p' = \frac{1}{\eta}$ and J_{KL}^{n+1} is defined in (3.13). Using definition (3.14), we obtain

$$\Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2 \geq \Lambda_{KL} (\phi(v_K^{n+1}) - \phi(v_L^{n+1}))^2,$$

and estimate (4.3) follows directly.

Let $T \in \mathcal{T}$, and let $(K, L) \in \mathcal{V}^2$, we use the notation:

$$\lambda_{KL}^T := -\int_T \Lambda \nabla e_K \cdot \nabla e_L dx = \lambda_{LK}^T, \tag{4.4}$$

so that $\Lambda_{KL} = \sum_{T \in \mathcal{T}} \lambda_{KL}^T$ for all $\sigma_{KL} \in \mathcal{E}$.

Lemma 4.3. Let $\Psi_{\mathcal{T}} = \sum_{K \in \mathcal{V}} \psi_K e_K \in V_{\mathcal{T}}$, then there exists a constant C_0 depending on Λ and $\theta_{\mathcal{T}}$ such that

$$\sum_{\sigma_{KL} \in \mathcal{E}} \sum_{T \in \mathcal{T}} |\lambda_{KL}^{T}| (\psi_K - \psi_L)^2 \le C_0 \int_{\Omega} \Lambda \nabla \Psi_{\mathcal{T}} \cdot \nabla \Psi_{\mathcal{T}} dx.$$
 (4.5)

Proof. We refer to [[13], Lemma 3.2] for the proof of this lemma.

Lemma 4.4. There exists a constant C_1 depending on Λ and θ_T such that

$$\sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} |\Lambda_{KL}| \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2 \le C_1 \sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2.$$

$$(4.6)$$

Proof. We refer to [[14], Lemma 3.3] for the proof of this lemma.

4.3. Entropy estimate on $v_{\mathcal{M},\Delta t}$.

Lemma 4.5. There exists C > 0 depending on $||v_0||_{L^2(\Omega)}$, Ω , T such that, for all $n^* \in \{0, \dots, N-1\}$,

$$\sum_{K \in \mathcal{V}} m_K \Gamma(v_K^{n^*+1}) + \sum_{n=0}^{n^*} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2 \leq C.$$

Proof. Since the function Γ defined in (3.10) is convex on (0,1), then by Jensen's inequality there holds

$$\Gamma\Big(\frac{1}{m_K}\int_{\omega_K}v_0(x)dx\Big) \leq \frac{1}{m_K}\int_{\omega_K}\Gamma(v_0(x))dx.$$

So

$$\sum_{K\in\mathcal{V}} m_K \Gamma(v_K^0) \leq \int_{\Omega} \Gamma(v_0(x)) dx.$$

Observing that $\Gamma(v) \leq (v-1)^2$ for $0 \leq v \leq 1$, one gets

$$\sum_{K \in \mathcal{V}} m_K \Gamma(v_K^0) \le \int_{\Omega} (v_0(x) - 1)^2 dx \le C. \tag{4.7}$$

Multiplying equation (3.12) by $p(v_K^{n+1})\Delta t$ and summing over $K \in \mathcal{V}$ and $n = 0, \dots, n^*$, we reach

$$T_1 + T_2 = T_3, (4.8)$$

where

$$T_1 := \sum_{n=0}^{n^*} \sum_{K \in \mathcal{V}} m_K (v_K^{n+1} - v_K^n) p(v_K^{n+1}),$$

$$T_2 := \sum_{n=0}^{n^*} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2,$$

and

$$T_3 := -\sum_{n=0}^{n^*} \Delta t \sum_{K \in \mathcal{V}} m_K I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) p(v_K^{n+1}).$$

Recalling (2.13) and that $\lim_{v\to 0^+} p(v) = -\infty$ and $\lim_{v\to 1^-} p(v) = \infty$, one can show that for $0 \le v \le 1$, there exists a positive constants c_2 , such that for all $w_j \in [0,1], j=1,\cdots,6$ and $c_m \le c \le c_M$, the function $-I_{\text{ion}}(v,\mathbf{w},c)p(v)$ verifies

$$-\infty < -I_{\text{ion}}(v, \mathbf{w}, c)p(v) < c_2.$$

As a result, one obtains

$$T_3 \le c_2 \sum_{n=0}^{n^*} \Delta t \sum_{K \in \mathcal{V}} m_K \le c_2 T |\Omega|.$$
 (4.9)

Since the function p is increasing, a convexity inequality gives

$$(a-b)p(a) \ge \Gamma(a) - \Gamma(b), \quad \forall (a,b) \in \mathbb{R}^+ \times \mathbb{R}^+,$$

providing

$$T_1 \ge \sum_{n=0}^{n^*} \sum_{K \in \mathcal{V}} m_K \Big(\Gamma(v_K^{n+1}) - \Gamma(v_K^n) \Big) = \sum_{K \in \mathcal{V}} m_K (\Gamma(v_K^{n^*+1}) - \Gamma(v_K^0) \Big). \tag{4.10}$$

Using estimates (4.10), (4.9) and (4.7) in equation (4.8), the proof of Lemma 4.5 is complete. \Box

We suggest to derive in the following lemma a classical energy estimate on $v_{\mathcal{T},\Delta t}$.

Lemma 4.6. There exists C depending on Ω , $||v_0||_{L^2(\Omega)}$ and T such that for all $n^* \in \{0, \dots, N-1\}$

$$\frac{1}{2} \sum_{K \in \mathcal{V}} m_K \left(v_K^{n^* + 1} \right)^2 + \sum_{n = 0}^{n^*} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} (v_K^{n+1} - v_L^{n+1})^2 \le C.$$

Proof. Let $n \in \{0, \dots, n^*\}$, then multiplying equation (3.12) by $v_K^{n+1} \Delta t$ and summing over $K \in \mathcal{V}$ provides

$$\mathcal{A} + \mathcal{B} = \mathcal{C} \tag{4.11}$$

where

$$\begin{split} \mathcal{A} := \sum_{K \in \mathcal{V}} m_K (v_K^{n+1} - v_K^n) v_K^{n+1}, \\ \mathcal{B} := \Delta t \sum_{K \in \mathcal{V}} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1})) (v_K^{n+1} - v_L^{n+1}), \end{split}$$

and

$$\mathcal{C} := -\Delta t \sum_{K \in \mathcal{V}} m_K \Big(I_{\text{Pot}}(v_K^{n+1}) + I_z(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_{Na}(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_s(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \Big) v_K^{n+1}.$$

The simple inequality $a(a-b) \ge \frac{a^2}{2} - \frac{b^2}{2}$ implies that

$$A \ge \frac{1}{2} \sum_{K \in \mathcal{V}} m_K (v_K^{n+1})^2 - \frac{1}{2} \sum_{K \in \mathcal{V}} m_K (v_K^n)^2.$$
(4.12)

It follows from definitions (3.14) of η_{KL}^{n+1} and (3.9) of p along with the mean value theorem that

$$\Lambda_{KL}^{n+1}\eta_{KL}^{n+1}(p(v_K^{n+1})-p(v_L^{n+1}))(v_K^{n+1}-v_L^{n+1}) \geq \Lambda_{KL}(v_K^{n+1}-v_L^{n+1})^2, \quad \forall \sigma_{KL} \in \mathcal{E}.$$

Hence,

$$\mathcal{B} \ge \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} (v_K^{n+1} - v_L^{n+1})^2. \tag{4.13}$$

Considering now the term C, note that by the maximum principle shown in Lemma 4.1 there exists a constant $c_1 > 0$ such that

$$\left| I_{\text{Pot}}(v_K^{n+1}) + I_z(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_{Na}(v_K^{n+1}, \mathbf{w}_K^{n+1}) + I_s(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \right| |v_K^{n+1}| \le c_1.$$

As a result, one obtains

$$C \le \Delta t |\Omega| c_1. \tag{4.14}$$

Using estimates (4.12),(4.13) and (4.14) in equation (4.11) and taking sums over $n \in \{0, \dots, N-1\}$ yields

$$\frac{1}{2} \sum_{K \in \mathcal{V}} m_K (v_K^{n^*+1})^2 + \sum_{n=0}^{n^*} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} (v_K^{n+1} - v_L^{n+1})^2 \le \frac{1}{2} \sum_{K \in \mathcal{V}} m_K (v_K^0)^2 + T |\Omega| c_1.$$

Finally, note that

$$\sum_{K \in \mathcal{V}} m_K (v_K^0)^2 \le |\Omega|,$$

to conclude the proof of Lemma 4.6.

4.4. Enhanced Estimates on $v_{\mathcal{M},\Delta t}$.

Lemma 4.7. Assume that $\int_{\Omega} v_0(x)dx > 0$, then there exists $\zeta > 0$ depending on the discretization and on the data such that

$$\int_{\Omega} v_{\mathcal{M},\Delta t} dx \ge \zeta, \qquad \forall t \in [0, T].$$

Proof. Multiplying equation (3.12) by Δt and taking sums over $K \in \mathcal{V}$ one gets

$$\sum_{K \in \mathcal{V}} m_K(v_K^{n+1} - v_K^n) = -\sum_{K \in \mathcal{V}} m_K \Delta t I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n). \tag{4.15}$$

One can use induction over n. Indeed, because of the assumption on the initial datum v_0 , there exists $L^{n_0} \in \mathcal{V}$ such that $v_{L^{n_0}}^0 > 0$. Assume that $v_{L^n}^n > 0$ for some $L^n \in \mathcal{V}$. Suppose that $\sum_{K \in \mathcal{V}} m_K v_K^{n+1} = 0$. Then by non-negativity of v_K^{n+1} and Equation (4.15), one deduces that $v_K^{n+1} = 0$, for all $K \in \mathcal{V}$ and that (recall (2.13))

$$\sum_{K \in \mathcal{V}} m_K v_K^n = \sum_{K \in \mathcal{V}} m_K \Delta t I_{\text{ion}}(0, \mathbf{w}_K^{n+1}, c_K^n) \le 0,$$

yielding a contradiction. Hence, there exists $L^{n+1} \in \mathcal{V}$ such that $v_{L^{n+1}}^{n+1}$ is strictly positive and

$$\sum_{K \in \mathcal{V}} m_K v_K^{n+1} := \zeta_{n+1} > 0.$$

Setting $\zeta = \min_{n=1,\dots,N} \zeta_n$, the proof is complete.

Lemma 4.8. Assume that $\int_{\Omega} (1 - v_0(x)) dx > 0$, then there exists $\rho > 0$ depending on the discretization and on the data such that

$$\int_{\Omega} (1 - v_{\mathcal{M}, \Delta t}) dx \ge \rho, \qquad \forall t \in [0, T].$$

Proof. Multiplying equation (3.12) by Δt and taking sums over $K \in \mathcal{V}$ one gets

$$\sum_{K \in \mathcal{V}} m_K(v_K^{n+1} - v_K^n) = -\sum_{K \in \mathcal{V}} m_K \Delta t I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n). \tag{4.16}$$

Again, one can use induction over n as in the proof of Lemma 4.7. Assume that $v_{L^n}^n > 0$ for some $L^n \in \mathcal{V}$, as this is the case for the initial datum v_0 . Suppose that $\forall K \in \mathcal{V}, v_K^{n+1} = 1$. Then by Equation (4.16), one deduces that

$$|\Omega| > \sum_{K \in \mathcal{V}} m_K v_K^n = |\Omega| - \sum_{K \in \mathcal{V}} m_K \Delta t I_{\text{ion}}(1, \mathbf{w}_K^{n+1}, c_K^n) \ge |\Omega|,$$

yielding a contradiction. Hence, there exists $L^{n+1} \in \mathcal{V}$ such that $v_{L^{n+1}}^{n+1} < 1$ and

$$\sum_{K \in \mathcal{V}} m_K v_K^{n+1} := |\Omega| - \rho_{n+1} < |\Omega|.$$

Setting $\rho = \min_{n=1,\dots,N} \rho_n$, the proof is complete.

Now we define the notion of transmissive path as introduced in [13].

Definition 4.1. A transmissive path \mathfrak{p} joining $K_i \in \mathcal{V}$ to $K_f \in \mathcal{V}$ consists in a list of vertices $(K_q)_{0 \leq q \leq M}$ such that $K_i = K_0$, $K_f = K_M$, with $K_q \neq K_\ell$ if $q \neq \ell$, and such that $\sigma_{K_qK_{q+1}} \in \mathcal{E}$ with $\Lambda_{K_qK_{q+1}} > 0$ for all $q \in \{0, ..., M-1\}$. We denote by $\mathbb{P}(K_i, K_f)$ the set of all transmissive paths joining $K_i \in \mathcal{V}$ to $K_f \in \mathcal{V}$.

We recall also a result proved in [13].

Lemma 4.9. For all $(K_i, K_f) \in \mathcal{V}^2$, there exists a transmissive path $\mathfrak{p} \in \mathbb{P}(K_i, K_f)$.

Proof. Let $K_i \in \mathcal{V}$, then define $\bar{\mathcal{V}}_{K_i}$ the subset of \mathcal{V} made of the vertices connected to K_i via a transmissive path. Note that $\bar{\mathcal{V}}_{K_i} \neq \emptyset$ since $\sum_{L \neq K} \Lambda_{KL} > 0$ and $\Lambda_{KM} = 0$ for all $M \notin \mathcal{V}_K$ (i.e. $\exists L \in \mathcal{V}_K$ such that $\Lambda_{KL} > 0$). Assume that $\bar{\mathcal{V}}_{K_i} \subsetneq \mathcal{V}$. Introduce the function $\psi_{\mathcal{T}} \in \mathcal{V}_{\mathcal{T}}$ such that

$$\psi_K = \begin{cases} 1 & \text{if } K \in \bar{\mathcal{V}}_{K_i} \\ 0 & \text{otherwise.} \end{cases}$$

The lack of transmissive path between the elements of $\bar{\mathcal{V}}_{K_i}$ and the elements of $\mathcal{V} \setminus \bar{\mathcal{V}}_{K_i}$ leads to

$$\sum_{\sigma_{KL} \in \mathcal{E}} (\Lambda_{KL})^+ (\psi_K - \psi_L)^2 = 0.$$

On the other hand, since $\bar{\mathcal{V}}_{K_i} \neq \emptyset$, the function $\psi_{\mathcal{T}}$ is not constant. Therefore, since Ω is assumed to be connected,

$$\sum_{\sigma_{KL} \in \mathcal{E}} (\Lambda_{KL})^{+} (u_K - u_L)^2 \ge \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} (u_K - u_L)^2 = \int_{\Omega} \Lambda \nabla u_{\mathcal{T}} \cdot \nabla u_{\mathcal{T}} dx > 0$$

providing a contradiction. The fact that the path is necessarily of finite length originates from the finite number of possible combinations for designing a path. \Box

Lemma 4.10. Assume that $\int_{\Omega} v_0(x)dx > 0$, then there exists $\kappa_h > 0$ depending on the data, the mesh \mathcal{T} and Δt such that

$$v_K^{n+1} \ge \kappa_h, \quad \forall K \in \mathcal{V}, \forall n \in \{0, \cdots, N-1\}.$$
 (4.17)

Proof. By Lemma 4.7, there exists K_i such that $v_{K_i}^{n+1} > 0$. Let $K_f \in \mathcal{V}$, then thanks to Lemma 4.9, there exists a transmissive path $\mathfrak{p} = (K_q)_{0 \leq q \leq M} \in \mathbb{P}(K_i, K_f)$, with $K_0 = K_i$ and $K_M = K_f$. Exploiting Lemma 4.4 and Lemma 4.5, one has the existence of C > 0 such that

$$\sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} |\Lambda_{KL}| \eta_{KL}^{n+1} \Big(p(v_K^{n+1}) - p(v_L^{n+1}) \Big)^2 \le C.$$

In particular, we get

$$\Lambda_{K_q K_{q+1}} \eta_{K_q K_{q+1}}^{n+1} \left(p(v_{K_q}^{n+1}) - p(v_{K_{q+1}}^{n+1}) \right)^2 \le \frac{C}{\Delta t}, \quad \forall q \in \{0, \cdots, M-1\}.$$

Assuming that $v_{K_q}^{n+1} > 0$, as this holds for q = 0, then $\eta_{K_q K_{q+1}}^{n+1} \ge \eta(v_{K_q}^{n+1}) > 0$. Then one has

$$\left(p(v_{K_q}^{n+1}) - p(v_{K_{q+1}}^{n+1})\right)^2 \leq \frac{C}{\Delta t \Lambda_{K_q K_{q+1}} \eta_{K_q K_{q+1}}^{n+1}} < \infty.$$

Hence, $p(v_{K_{q+1}}^{n+1}) > -\infty$ and $v_{K_{q+1}}^{n+1} > 0$. By a straightforward induction, one can obtain that $v_{K_f}^{n+1} > 0$ and since K_f is arbitrary, one gets that

$$v_K^{n+1} > 0, \quad \forall K \in \mathcal{V}.$$

Keeping in mind that the set $\mathcal{V} \times \{0, \dots, N-1\}$ is finite, one deduces the existence of $\kappa_h > 0$ such that (4.17) holds.

Similarly, one can prove the following.

Lemma 4.11. Assume that $\int_{\Omega} (1-v_0(x))dx > 0$, then there exists $\rho_h > 0$ depending on the data, the mesh \mathcal{T} and Δt such that

$$v_K^{n+1} \le 1 - \rho_h, \quad \forall K \in \mathcal{V}, \forall n \in \{0, \dots, N-1\}.$$
 (4.18)

4.5. Energy estimates on $w_{\mathcal{T},\Delta t}$ and $c_{\mathcal{T},\Delta t}$.

Definition 4.2. For all $(K, L) \in \mathcal{V}^2$, define ξ_{KL} by

$$\xi_{KL} = -\int_{\Omega} \nabla e_K \cdot \nabla e_L dx.$$

Lemma 4.12. Let $(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^{n+1})_{K \in \mathcal{V}, n \in \{0, \dots, N\}}$ be a solution of the discrete scheme (3.12), (3.6), (3.7). Assume that $\xi_{KL} \geq 0$ for all $(K, L) \in \mathcal{V}$, then there exist constants C_2 , and $C_3 > 0$ depending on Ω , T, v_0 , w_0 , c_0 such that

$$\|\nabla w_{j,\tau}\|_{L^2(\Omega_T)}^2 = \sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \xi_{KL} |w_{j,L}^{n+1} - w_{j,K}^{n+1}|^2 \le C_2, \quad \forall j = 1, \dots, 6,$$
 (4.19)

and

$$\|\nabla c_{\mathcal{T}}\|_{L^{2}(\Omega_{T})}^{2} = \sum_{n=0}^{N-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \xi_{KL} |c_{L}^{n+1} - c_{K}^{n+1}|^{2} \le C_{3}.$$

$$(4.20)$$

Remark 4.1. Note that if all the angles in the primal triangular mesh are acute then the above assumption $(\xi_{KL} \geq 0 \text{ for all } (K, L) \in \mathcal{V})$ is fulfilled.

Proof. In order to prove estimate (4.19), we drop the index j to simplify the notation, and we consider equation (3.6) separately on the vertices K and L. Subtracting the two equations, there holds for all $L \in \mathcal{V}_K$:

$$\frac{w_K^{n+1} - w_L^{n+1}}{\Delta t} - \frac{w_K^n - w_L^n}{\Delta t} = \left(\alpha(v_K^n) - \alpha(v_L^n)\right) (1 - w_K^{n+1}) - \left(\alpha(v_L^n) + \beta(v_L^n)\right) (w_K^{n+1} - w_L^{n+1}) - \left(\beta(v_K^n) - \beta(v_L^n)\right) w_K^{n+1}$$

Multiplying both sides of the equation by $w_K^{n+1} - w_L^{n+1}$, then noting that $1 - w_K^{n+1} \le 1$, $w_K^{n+1} \le 1$ and $(\alpha(v_L^n) + \beta(v_L^n)) \ge 0$, one gets

$$(w_K^{n+1} - w_L^{n+1}) \Big(\frac{w_K^{n+1} - w_L^{n+1}}{\Delta t} - \frac{w_K^n - w_L^n}{\Delta t} \Big) \quad \leq \quad \Big| \alpha(v_K^n) - \alpha(v_L^n) \Big| |w_K^{n+1} - w_L^{n+1}| \\ \qquad \qquad + \Big| \beta(v_K^n) - \beta(v_L^n) \Big| |w_K^{n+1} - w_L^{n+1}|,$$

and by Young's inequality with $\varepsilon = \frac{1}{2}$, we get:

$$(w_K^{n+1} - w_L^{n+1}) \left(\frac{w_K^{n+1} - w_L^{n+1}}{\Delta t} - \frac{w_K^n - w_L^n}{\Delta t} \right) \leq \frac{1}{2} \left| \alpha(v_K^n) - \alpha(v_L^n) \right|^2 + \frac{1}{2} \left| \beta(v_K^n) - \beta(v_L^n) \right|^2 + |w_K^{n+1} - w_L^{n+1}|^2.$$

Now using the inequality $a(a-b) \ge \frac{1}{2}(a^2-b^2)$ on the left hand side of the above inequality we obtain:

$$\frac{1}{2\Delta t} \Big((w_K^{n+1} - w_L^{n+1})^2 - (w_K^n - w_L^n)^2 \Big) \leq \frac{1}{2} \Big| \alpha(v_K^n) - \alpha(v_L^n) \Big|^2 + \frac{1}{2} \Big| \beta(v_K^n) - \beta(v_L^n) \Big|^2 + |w_K^{n+1} - w_L^{n+1}|^2.$$

By the regularity of α and β and the confinement of v_K^n , there exists a constant $c_3 > 0$ such that:

$$\frac{1}{\Delta t} \Big((w_K^{n+1} - w_L^{n+1})^2 - (w_K^n - w_L^n)^2 \Big) \le c_3 (v_K^n - v_L^n)^2 + 2|w_K^{n+1} - w_L^{n+1}|^2.$$

By the discrete differential form of Gronwall's inequality (see for instance [17]), one has:

$$(w_K^n - w_L^n)^2 \le (1 - 2\Delta t)^{-n} \Big((w_K^0 - w_L^0)^2 + c_3 \Delta t \sum_{j=0}^{n-1} (1 - 2\Delta t)^j (v_K^j - v_L^j)^2 \Big).$$

Note that for $\Delta t \leq 1/2$, we have

$$(w_K^n - w_L^n)^2 \le e^{2T} \Big((w_K^0 - w_L^0)^2 + c_3 \Delta t \sum_{j=0}^{n-1} (v_K^j - v_L^j)^2 \Big).$$

Multiplying both sides by ξ_{KL} and taking sums, one gets:

$$\sum_{\sigma_{KL} \in \mathcal{E}} \xi_{KL} (w_K^n - w_L^n)^2 \leq e^{2T} \Big(\|\nabla w_T^0\|_{L^2(\Omega)}^2 + c_3 \sum_{j=0}^{n-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \xi_{KL} (v_K^j - v_L^j)^2 \Big).$$

Now using Lemma 4.6, we get:

$$\sum_{\sigma_{KL} \in \mathcal{E}} \xi_{KL} (w_K^n - w_L^n)^2 \le e^{2T} \Big(\|\nabla w_T^0\|_{L^2(\Omega)}^2 + c_3 C \Big),$$

leading to

$$\sum_{n=1}^{N} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \xi_{KL} (w_K^n - w_L^n)^2 \le T e^{2T} \Big(\|\nabla w_T^0\|_{L^2(\Omega)}^2 + c_3 C \Big).$$

Thus estimate (4.19) is obtained.

To obtain estimate (4.20) the above argument is repeated. Consider equation (3.7) on the vertices K and L, then subtract the resulting equations to get for $L \in \mathcal{V}_K$:

$$\frac{c_K^{n+1} - c_L^{n+1}}{\Delta t} - \frac{c_K^n - c_L^n}{\Delta t} = -0.07(c_K^{n+1} - c_L^{n+1}) - g_s 10^{-4} \left(-7.7(f_K^{n+1} r_K^{n+1} - f_L^{n+1} d_L^{n+1}) + 13.0287(f_K^{n+1} r_K^{n+1} \ln(c_K^{n+1}) - f_L^{n+1} r_L^{n+1} \ln(c_L^{n+1})) + f_K^{n+1} r_K^{n+1} v_K^{n+1} - f_L^{n+1} r_L^{n+1} v_L^{n+1} \right).$$

For simplicity, we write the above equation as:

$$\frac{c_K^{n+1}-c_L^{n+1}}{\Delta t}-\frac{c_K^n-c_L^n}{\Delta t}=-0.07(c_K^{n+1}-c_L^{n+1})-(H(v_K^{n+1},f_K^{n+1},r_K^{n+1},c_K^{n+1})-H(v_L^{n+1},f_L^{n+1},r_L^{n+1},c_L^{n+1})),$$

where

$$H(v, f, r, c) = g_s 10^{-4} fr(v - 7.7 + 13.0287 \ln(c)).$$

Multiplying both sides by $(c_K^{n+1} - c_L^{n+1})$ then applying Young's inequality, we get:

$$(c_K^{n+1} - c_L^{n+1}) \Big(\frac{c_K^{n+1} - c_L^{n+1}}{\Delta t} - \frac{c_K^n - c_L^n}{\Delta t} \Big) \leq 0.57 (c_K^{n+1} - c_L^{n+1})^2$$

$$+ \frac{1}{2} \Big(H(v_K^{n+1}, f_K^{n+1}, r_K^{n+1}, c_K^{n+1}) - H(v_L^{n+1}, f_L^{n+1}, r_L^{n+1}, c_L^{n+1}) \Big)^2.$$

Using the regularity of H and the maximum principle (in particular, $c_K^n \ge c_m > 0$), we can find a constant $C_H > 0$ such that:

$$(c_K^{n+1} - c_L^{n+1}) \left(\frac{c_K^{n+1} - c_L^{n+1}}{\Delta t} - \frac{c_K^n - c_L^n}{\Delta t} \right) \leq 0.57 (c_K^{n+1} - c_L^{n+1})^2 + \frac{C_H}{2} \left((v_K^{n+1} - v_L^{n+1})^2 + (f_K^{n+1} - f_L^{n+1})^2 + (f_K^{n+1} - f_L^{n+1})^2 + (f_K^{n+1} - f_L^{n+1})^2 + (f_K^{n+1} - f_L^{n+1})^2 \right),$$

and by the inequality $a(a-b) \ge \frac{1}{2}(a^2-b^2)$, we get:

$$\frac{(c_K^{n+1} - c_L^{n+1})^2 - (c_K^n - c_L^n)^2}{\Delta t} \leq 1.14(c_K^{n+1} - c_L^{n+1})^2 + (c_K^{n+1} - c_L^{n+1})$$

So we have

$$\frac{(c_K^{n+1} - c_L^{n+1})^2 - (c_K^n - c_L^n)^2}{\Delta t} \le (1.14 + C_H)(c_K^{n+1} - c_L^{n+1})^2 + C_H \left((v_K^{n+1} - v_L^{n+1})^2 + (f_K^{n+1} - f_L^{n+1})^2 + (r_K^{n+1} - r_L^{n+1})^2 \right).$$

Estimate (4.20) follows easily from this last inequality by using Gronwall's inequality provided that $\Delta t \leq \frac{1}{1.14 + C_H}$ by a similar argument to the one used in the case of proving (4.19). Therefore the proof of the lemma is complete.

Now, we state some estimates obtained on the discrete evolutive terms of the gating and concentration variables.

Lemma 4.13. Let $(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^{n+1})_{K \in \mathcal{V}, n \in \{0, \dots, N\}}$ be a solution of the discrete scheme (3.12), (3.6), (3.7). Then there exist constants C_4 , and $C_5 > 0$ depending on Ω , T such that

$$\sum_{n=0}^{N-1} \Delta t \sum_{K \in \mathcal{V}} m_K \left(\frac{w_{j,K}^{n+1} - w_{j,K}^n}{\Delta t} \right)^2 \le C_4, \quad \forall j = 1, \dots, 6,$$
(4.21)

and

$$\sum_{n=0}^{N-1} \Delta t \sum_{K \in \mathcal{V}} m_K \left(\frac{c_K^{n+1} - c_K^n}{\Delta t} \right)^2 \le C_5.$$
 (4.22)

Proof. Consider equation (3.6) (dropping the index j for simplicity), multiply it by $m_K \frac{w_K^{n+1} - w_K^n}{(\Delta t)^2}$ then sum over all $K \in \mathcal{V}$ and make use of Lemma 4.1 to easily obtain estimate (4.21). Estimate (4.22) is obtained similarly by multiplying equation (3.7) by $m_K \frac{c_K^{n+1} - c_K^n}{(\Delta t)^2}$.

4.6. Existence of a discrete solution.

Proposition 4.1. Under the assumptions on the model stated in Section 2, there exists at least one solution $(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^{n+1})_{K \in \mathcal{V}}$ of the scheme (3.12), (3.7), (3.6).

Proof. We show existence of a discrete solution using induction over n. We assume that $(v_K^n, \mathbf{w}_K^n, c_K^n)_{K \in \mathcal{V}}$ exists and we prove the existence of $(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^{n+1})_{K \in \mathcal{V}}$.

Using equation (3.6), we get for each $j=1,\dots,6$, and for all $K\in\mathcal{V}$ the explicit expression of $w_{i,K}^{n+1}$ as:

$$w_{j,K}^{n+1} = \frac{w_{j,K}^n + \Delta t(\alpha_j(v_K^n))}{1 + \Delta t(\alpha_j(v_K^n) + \beta_j(v_K^n))},$$

and hence $(\mathbf{w}_K^{n+1})_{K\in\mathcal{V}}$ exists since $\alpha_j, \beta_j > 0$. Now, we consider equation (3.12) and we assume that $(v_K^n)_{K\in\mathcal{V}}$ and $(w_K^{n+1})_{K\in\mathcal{V}}$ exist. The existence of a solution $(v_K^{n+1})_{K\in\mathcal{V}}$ can be proved by a slight modification of the proof of Proposition 3.11 in [13] or Proposition 3.12 in [14], which rely on a topological degree argument.

Let $\mu \in [0,1]$, we denote by $(v_{K,\mu}^{n+1})_{K \in \mathcal{V}}$ the solution of the scheme:

$$\frac{m_K}{\Delta t}(v_{K,\mu}^{n+1} - v_K^n) + \mu \sum_{\sigma_{KL} \in \mathcal{E}_K} \Lambda_{KL} \eta_{KL,\mu}^{n+1} \Big(p(v_{K,\mu}^{n+1}) - p(v_{L,\mu}^{n+1}) \Big) \\
+ (1 - \mu) \sum_{\sigma_{KL} \in \mathcal{E}_K} |\Lambda_{KL}| \Big(p(v_{K,\mu}^{n+1}) - p(v_{L,\mu}^{n+1}) \Big) = -m_K I_{\text{ion}}(v_{K,\mu}^{n+1}, \mathbf{w}_K^{n+1}, c_K^n), \tag{4.23}$$

where

$$\eta_{KL,\mu}^{n+1} = \left\{ \begin{array}{ll} \max_{v \in J_{KL,\mu}^{n+1}} \eta(v) & \text{if } \Lambda_{KL} \geq 0, \\ \min_{v \in J_{KL,\mu}^{n+1}} \eta(v) & \text{if } \Lambda_{KL} < 0, \end{array} \right.$$

and $J_{KL,\mu}^{n+1} = \left[\min(v_{K,\mu}^{n+1},v_{L,\mu}^{n+1}),\max(v_{K,\mu}^{n+1},v_{L,\mu}^{n+1})\right]$. Carefully reproducing the analysis carried out in Lemma 4.2 and Lemma 4.5, one can show that for all $\mu \in [0,1]$,

$$\sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} \left(\phi(v_{K,\mu}^{n+1}) - \phi(v_{L,\mu}^{n+1}) \right)^2 \le \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} \eta_{KL,\mu}^{n+1} \left(p(v_{K,\mu}^{n+1}) - p(v_{L,\mu}^{n+1}) \right)^2 \le C. \tag{4.24}$$

Furthermore, one can prove as in Lemma 4.1 that

$$0 \le v_{K,u}^{n+1} \le 1$$
,

and this last estimate can be enhanced as in § 4.4 that there exists $\epsilon > 0$ such that

$$0 < \epsilon \le v_{K,\mu}^{n+1} \le 1 - \epsilon < 1, \qquad \forall K \in \mathcal{V}. \tag{4.25}$$

As a result, for all $\mu \in [0,1]$, the solutions of the numerical scheme (4.23) are kept in the interior of a compact subset $\mathcal B$ of $[0,1]^{\operatorname{Card}(\mathcal V)}$ such that

$$\operatorname{dist}\left(\mathcal{B}, \{0,1\}^{\operatorname{Card}(\mathcal{V})}\right) \ge \frac{\epsilon}{2}.$$

Define the function $\Xi : \mathcal{B} \times [0,1] \to \mathbb{R}^{\operatorname{Card}(\mathcal{V})}$ by: $\forall K \in \mathcal{V}$,

$$\Xi_{K}((u_{K})_{K}, \mu) := \frac{m_{K}}{\Delta t}(u_{K} - v_{K}^{n}) + \mu \sum_{\sigma_{KL} \in \mathcal{E}_{K}} \Lambda_{KL} \eta_{KL,\mu}^{n+1} \Big(p(u_{K}) - p(u_{L}) \Big) + (1 - \mu) \sum_{\sigma_{KL} \in \mathcal{E}_{K}} |\Lambda_{KL}| \Big(p(u_{K}) - p(u_{L}) \Big) + m_{K} I_{\text{ion}}(u_{K}, \mathbf{w}_{K}^{n+1}, c_{K}^{n}).$$

The function Ξ is uniformly continuous on $\mathcal{B} \times [0,1]$, and it follows from (4.25) that for all $\mu \in [0,1]$ the solution $(v_{K,\mu}^{n+1})_{K\in\mathcal{V}}$ of the nonlinear system

$$\Xi\left(\left(v_{K,\mu}^{n+1}\right)_{K\in\mathcal{V}},\mu\right)=0,\tag{4.26}$$

cannot reach $\partial \mathcal{B}$. Therefore the topological degree $\delta(\Xi,\mathcal{B})(\mu)$ is constant with respect to μ . For $\mu = 0$, the system (4.26) is monotone and it can be proved that its topological degree is equal to 1 (by adapting the existence proof of a discrete solution to the monotone implicit scheme for a hyperbolic equation studied in [19]). Hence, it admits at least one solution for $\mu = 1$, establishing the existence of $\left(v_K^{n+1}\right)_{K\in\mathcal{V}}$. Now given v_K^{n+1} and w_K^{n+1} , we can rewrite Equation (3.7) as:

$$(1+0.07\Delta t)c_K^{n+1} + 13.0287 \times 10^{-4}g_s f_K^{n+1} r_K^{n+1} \ln(c_K^{n+1}) = c_K^n + 10^{-4} \Delta t \Big(0.07 - g_s w_K^{n+1} (v_K^{n+1} - 7.7)\Big). \tag{4.27}$$

Since the function $x \mapsto (1+0.07\Delta t)x+13.0287\times 10^{-4}g_sf_K^{n+1}r_K^{n+1}\ln(x)$, which is defined for x>0 onto \mathbb{R} , is bijective. Thus, Equation (4.27) admits a unique solution c_K^{n+1} . Therefore, the existence of solution of the discrete system is obtained.

5. Compactness estimates on the family of discrete solutions

The sequences $\left(v_{\mathcal{M}_m,\Delta t_m}\right)_m$, $\left(\mathbf{w}_{\mathcal{M}_m,\Delta t_m}\right)_m$, $\left(c_{\mathcal{M}_m,\Delta t_m}\right)_m$, $\left(v_{\mathcal{T}_m,\Delta t_m}\right)_m$, $\left(\mathbf{w}_{\mathcal{T}_m,\Delta t_m}\right)_m$, and $\left(c_{\mathcal{T}_m,\Delta t_m}\right)_m$ are uniformly bounded w.r.t m in $L^{\infty}(\Omega_T)$ as implied by Lemma 4.1. Moreover, as a consequence of Lemma 4.6, equation (3.3) and condition (2.1), the sequence $\left(v_{\mathcal{T}_m,\Delta t_m}\right)_m$ is uniformly bounded in $L^2(0,T;H^1(\Omega))$. Therefore, there exists $v \in L^2(0,T;H^1(\Omega))$ such that, up to a subsequence,

$$v_{\mathcal{T}_m,\Delta t_m} \to v$$
 weakly in $L^2(0,T;H^1(\Omega))$ as $m \to \infty$.

Using the inequality

$$||u_{\mathcal{T}_{m},\Delta t_{m}} - u_{\mathcal{M}_{m},\Delta t_{m}}||_{L^{2}(\Omega)} \leq Ch||\nabla u_{\mathcal{T}_{m},\Delta t_{m}}||_{L^{2}(\Omega)}, \quad \forall u_{\mathcal{T}_{m},\Delta t_{m}} \in \mathcal{H}_{\mathcal{T}_{m},\Delta t_{m}},$$
(see for example [11] Lemma 3.4), one deduces that $v_{\mathcal{T}_{m},\Delta t_{m}}$ and $v_{\mathcal{M}_{m},\Delta t_{m}}$ have the same limits, and

$$v_{\mathcal{M}_m,\Delta t_m} \to v$$
 weak-* in $L^{\infty}(\Omega_T)$.

On the other hand, making use of Lemma 4.12 the sequences $\left(\mathbf{w}_{\mathcal{T}_m,\Delta t_m}\right)_m$, and $\left(c_{\mathcal{T}_m,\Delta t_m}\right)_m$ are uniformly bounded in $L^2(0,T;(H^1(\Omega))^6)$ and $L^2(0,T;H^1(\Omega))$ respectively. Hence, there exist $\mathbf{w} \in L^2(0,T;((H^1(\Omega))^6))$ and $c \in L^2(0,T;H^1(\Omega))$ such that, up to a subsequence,

$$\mathbf{w}_{\mathcal{T}_m,\Delta t_m} \to \mathbf{w}$$
 weakly in $L^2(0,T;(H^1(\Omega))^6)$ as $m \to \infty$, $c_{\mathcal{T}_m,\Delta t_m} \to c$ weakly in $L^2(0,T;H^1(\Omega))$ as $m \to \infty$,

$$\mathbf{w}_{\mathcal{M}_m,\Delta t_m} \to \mathbf{w} \text{ weak-* in } (L^{\infty}(\Omega_T))^6$$

and

$$c_{\mathcal{M}_m, \Delta t_m} \to c$$
 weak-* in $L^{\infty}(\Omega_T)$.

In order to establish the convergence of the scheme, it is required to prove that

$$v_{\mathcal{M}_m,\Delta t_m} \to v$$
, $c_{\mathcal{M}_m,\Delta t_m} \to c$ and $\mathbf{w}_{\mathcal{M}_m,\Delta t_m} \to \mathbf{w}$ a.e. in Ω_T .

One option is to proceed in estimating the time and space translates of the discrete functions $v_{\mathcal{M}_m,\Delta t_m}$, $\mathbf{w}_{\mathcal{M}_m,\Delta t_m}$ and $c_{\mathcal{M}_m,\Delta t_m}$ as in [1] and [20]. The other alternative which we adopt herein is to make use of the technical blackbox proposed in Theorem 3.9 in [2].

First, note that Lemma (4.13) provides a discrete $L^2(0,T;L^2(\Omega))$ estimate on the time finite differences of $\mathbf{w}_{\mathcal{M}_m,\Delta t_m}$ and $c_{\mathcal{M}_m,\Delta t_m}$. Second, for a fixed $m \geq 1$, consider a set of nodal values $\left(\varphi_K^{n+1}\right)_{K \in \mathcal{V}_m, 0 \leq n \leq N_m - 1}$ such that $\varphi_K^{n+1} = 0$ if $x_K \in \partial\Omega$ and the corresponding functions $\varphi_{\mathcal{T}_m,\Delta t_m}$

and $\varphi_{\mathcal{M}_m,\Delta t_m}$. We have the following discrete $L^1(0,T;H^{-1}(\Omega))$ estimate on the finite difference w.r.t time of $v_{\mathcal{M}_m,\Delta t_m}$.

Lemma 5.1. There exists C independent of m such that

$$\sum_{n=0}^{N_m - 1} \sum_{K \in \mathcal{V}_m} m_K (v_K^{n+1} - v_K^n) \varphi_K^{n+1} \le C \|\nabla \varphi_{\mathcal{T}_m, \Delta t_m}\|_{L^2(\Omega_T)}.$$
 (5.2)

Proof. Multiply (3.12) by $\Delta t \varphi_K^{n+1}$ and sum over $n \in \{0, \dots, N_m - 1\}$ and $K \in \mathcal{V}_m$ to get

$$\sum_{n=0}^{N_m-1} \sum_{K \in \mathcal{V}_m} m_K (v_K^{n+1} - v_K^n) \varphi_K^{n+1} \le T_{1,m} + T_{2,m}, \tag{5.3}$$

where

$$T_{1,m} = -\sum_{n=0}^{N_m-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} \Lambda_{KL} \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1})) (\varphi_K^{n+1} - \varphi_L^{n+1}),$$

$$T_{2,m} = -\sum_{n=0}^{N_m-1} \Delta t \sum_{K \in \mathcal{V}_m} m_K I_{\text{ion}} (v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \varphi_K^{n+1}.$$

Applying Cauchy-Schwarz inequality and observing that $0 \le \eta \le 1$, there holds

$$|T_{1,m}|^2 \le \Big(\sum_{n=0}^{N_m-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} |\Lambda_{KL}| \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2 \Big) \Big(\sum_{n=0}^{N_m-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} |\Lambda_{KL}| (\varphi_K^{n+1} - \varphi_L^{n+1})^2 \Big).$$

The combined use of Lemma 4.3 and Lemma 4.5 implies

$$\sum_{n=0}^{N_m-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} |\Lambda_{KL}| \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2 \le C,$$

whereas Lemma 4.3 provides

$$\sum_{n=0}^{N_m-1} \Delta t \sum_{\sigma_{KL} \in \mathcal{E}} |\Lambda_{KL}| (\varphi_K^{n+1} - \varphi_L^{n+1})^2 \le C \|\nabla \varphi_{\mathcal{T}_m, \Delta t_m}\|_{L^2(\Omega_T)}^2.$$

Hence,

$$|T_{1,m}| \le C \|\nabla \varphi_{\mathcal{T}_m, \Delta t_m}\|_{L^2(\Omega_T)}.$$
(5.4)

Moreover, applying Cauchy-Schwarz inequality on $T_{2,m}$, on gets

$$|T_{2,m}| \le \left(\sum_{n=0}^{N_m-1} \Delta t \sum_{K \in \mathcal{V}_m} m_K \Big| I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \Big| \right)^{1/2} \|\varphi_{\mathcal{M}_m, \Delta t_m}\|_{L^2(\Omega_T)}.$$

Lemma 4.1 implies that

$$\left(\sum_{n=0}^{N_m-1} \Delta t \sum_{K \in \mathcal{V}_m} m_K \left| I_{\text{ion}}(v_K^n, \mathbf{w}_K^{n+1}, c_K^n) \right| \right)^{1/2} \le C,$$

whereas the discrete Poincaré inequality (see for instance Lemma 3.3 in [11]) provides

$$\|\varphi_{\mathcal{M}_m,\Delta t_m}\|_{L^2(\Omega_T)} \le C \|\nabla \varphi_{\mathcal{T}_m,\Delta t_m}\|_{L^2(\Omega_T)}.$$

As a result, one gets

$$|T_{2,m}| \le C \|\nabla \varphi_{\mathcal{T}_m, \Delta t_m}\|_{L^2(\Omega_T)}.$$
(5.5)

Plugging estimates (5.3) and (5.4) in inequality (5.5) ends the proof of estimate (5.2).

We have now all the necessary machinery to use Theorem 3.9 in [2], allowing us to claim that $v_{\mathcal{M}_m,\Delta t_m} \to v$ a.e. in Ω_T , $\mathbf{w}_{\mathcal{M}_m,\Delta t_m} \to \mathbf{w}$ a.e. in Ω_T and $c_{\mathcal{M}_m,\Delta t_m} \to c$ a.e. in Ω_T .

6. Identification of the limit as a weak solution

It remains to show that the limit (v, \mathbf{w}, c) satisfies the weak formulation (2.15)-(2.17). Consider a test function $\psi \in \mathcal{D}(\bar{\Omega} \times [0, T))$ and denote $\psi(x_K, t_n)$ by ψ_K^n for all $K \in \mathcal{V}_m$ and all $n \in \{0, \dots, N_m\}$. We prove in what follows the convergence of equation (3.12) of the scheme, i.e. we prove that equation (2.15) is satisfied when $m \to \infty$. The convergence of the other two equations, being standard, is left to the reader.

Multiplying equation (3.12) by $\Delta t_m \psi_K^n$ and summing over $n \in \{0, \dots, N_m - 1\}$ and $K \in \mathcal{V}_m$ yields:

$$A_m + D_{1,m} + D_{2,m} = R_m,$$

where

$$\begin{split} A_m &= \sum_{n=0}^{N_m-1} \sum_{K \in \mathcal{V}_m} m_K (v_K^{n+1} - v_K^n) \psi_K^n \\ D_{1,m} &= \sum_{n=0}^{N_m-1} \Delta t_m \sum_{\sigma_{KL} \in \mathcal{E}_m} \Lambda_{KL} \Big(\eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1})) - \sqrt{\eta_{KL}^{n+1}} (\phi(v_K^{n+1}) - \phi(v_L^{n+1})) \Big) (\psi_K^n - \psi_L^n) \\ D_{2,m} &= \sum_{n=0}^{N_m-1} \Delta t_m \sum_{\sigma_{KL} \in \mathcal{E}_m} \Lambda_{KL} \sqrt{\eta_{KL}^{n+1}} \Big(\phi(v_K^{n+1}) - \phi(v_L^{n+1}) \Big) (\psi_K^n - \psi_L^n) \\ R_m &= -\sum_{n=0}^{N_m-1} \Delta t_m \sum_{K \in \mathcal{V}} m_K I_{\text{ion}} (v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \psi_K^n. \end{split}$$

Accumulation term

Using integration by parts in time and keeping in mind that $\psi_K^{N_m} = 0$ for all $K \in \mathcal{V}_m$, notice that A_m can be written as:

$$A_{m} = \sum_{n=0}^{N_{m}-1} \sum_{K \in \mathcal{V}_{m}} m_{k} (v_{K}^{n+1} - v_{K}^{n}) \psi_{K}^{n}$$

$$= -\sum_{n=0}^{N_{m}-1} \Delta t_{m} \sum_{K \in \mathcal{V}_{m}} m_{K} v_{K}^{n+1} \frac{\psi_{K}^{n+1} - \psi_{K}^{n}}{\Delta t_{m}} - \sum_{K \in \mathcal{V}_{m}} m_{K} v_{K}^{0} \psi_{K}^{0}$$

$$= -\iint_{\Omega_{T}} v_{\mathcal{M}_{m}, \Delta t_{m}}(t, x) \partial_{t} \psi_{\mathcal{M}_{m}, \Delta t_{m}}(t, x) dx dt - \int_{\Omega} v_{\mathcal{M}_{m}, \Delta t_{m}}(0, x) \psi_{\mathcal{M}_{m}, \Delta t_{m}}(0, x) dx.$$

By regularity of ψ , and the convergence in $L^1(\Omega_T)$ of the sequence $(v_{\mathcal{M}_m,\Delta t_m})_m$ towards v, one obtains:

$$A_m \to -\iint_{\Omega_T} v(t, x) \partial_t \psi(t, x) dx dt - \int_{\Omega} v(0, x) \psi(0, x) dx$$
, as $m \to \infty$.

Diffusion term

It is required to prove that $\lim_{m\to\infty} D_{1,m} = 0$, and $\lim_{m\to\infty} D_{2,m} = \iint_{\Omega_T} \Lambda \nabla v \cdot \nabla \psi dx dt$. Let us prove first that $\lim_{m\to\infty} D_{1,m} = 0$.

For all $\sigma_{KL} \in \mathcal{E}_m$ and all $n \in \{0, \dots, N_m - 1\}$, denote by $\bar{\eta}_{KL}^{n+1}$ the following quantity:

$$\bar{\eta}_{KL}^{n+1} = \begin{cases} \left(\frac{\phi(v_K^{n+1}) - \phi(v_L^{n+1})}{p(v_K^{n+1}) - p(v_L^{n+1})}\right)^2 & \text{if } v_K^{n+1} \neq v_L^{n+1} \\ \eta\left(v_K^{n+1}\right) & \text{if } v_K^{n+1} = v_L^{n+1} \end{cases}$$

Then the term $D_{1,m}$ is rewritten as:

$$D_{1,m} = \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{\sigma_{KL} \in \mathcal{E}_m} \Lambda_{KL} \sqrt{\eta_{KL}^{n+1}} \left(\sqrt{\eta_{KL}^{n+1}} - \sqrt{\bar{\eta}_{KL}^{n+1}} \right) \left(p(v_K^{n+1}) - p(v_L^{n+1}) \right) (\psi_K^n - \psi_L^n).$$

An application of Cauchy-Schwarz' inequality yields

$$|D_{1,m}| \le \Big(\sum_{n=0}^{N_m-1} \Delta t_m \sum_{\sigma_{KL} \in \mathcal{E}_m} |\Lambda_{KL}| \eta_{KL}^{n+1} (p(v_K^{n+1}) - p(v_L^{n+1}))^2 \Big)^{1/2} \times P_m^{1/2},$$

where P_m is given by:

$$P_{m} = \sum_{n=0}^{N_{m}-1} \Delta t_{m} \sum_{\sigma_{KL} \in \mathcal{E}_{m}} |\Lambda_{KL}| \left(\sqrt{\eta_{KL}^{n+1}} - \sqrt{\bar{\eta}_{KL}^{n+1}} \right)^{2} (\psi_{K}^{n} - \psi_{L}^{n})^{2}.$$

Exploiting Lemma 4.4 and Lemma 4.5, one has $D_{1,m} \leq C P_m^{1/2}$. So, it is enough to show that $\lim_{m\to\infty} P_m = 0$ in order to obtain $\lim_{m\to\infty} D_{1,m} = 0$. For all $T \in \mathcal{T}_m$, we introduce the notations:

$$\bar{\phi}_T^{n+1} = \max_{x \in T} \left(\phi_{\mathcal{T}_m, \Delta t_m}(v)(t_{n+1}, x) \right), \quad \underline{\phi}_T^{n+1} = \min_{x \in T} \left(\phi_{\mathcal{T}_m, \Delta t_m}(v)(t_{n+1}, x) \right),$$

and for all $(t,x) \in (t_n,t_{n+1}) \times T$

$$\bar{\phi}_{\mathcal{T}_m,\Delta t_m}(t,x) = \bar{\phi}_T^{n+1}, \quad \underline{\phi}_{\mathcal{T}_m,\Delta t_m}(t,x) = \underline{\phi}_T^{n+1}.$$

Now for all $\sigma_{KL} \in \mathcal{E}_T$, there holds

$$\left| \sqrt{\eta_{KL}^{n+1}} - \sqrt{\bar{\eta}_{KL}^{n+1}} \right| \le \mu \left(\bar{\phi}_T^{n+1} - \underline{\phi}_T^{n+1} \right), \tag{6.1}$$

where μ is the continuity modulus of $\sqrt{\eta \circ \phi^{-1}}$. Indeed, the continuity and boundedness of $\sqrt{\eta \circ \phi^{-1}}$ on the interval $[\phi(0), \phi(1)]$ ensure the existence and boundedness of the continuity modulus μ . Therefore,

$$0 \le P_m \le \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{T \in \mathcal{T}_m} \mu \left(\bar{\phi}_T^{n+1} - \underline{\phi}_T^{n+1} \right)^2 \sum_{\sigma_{KL} \in \mathcal{E}_T} |\lambda_{KL}^T| (\psi_K^n - \psi_L^n)^2, \tag{6.2}$$

where λ_{KL}^T is defined by (4.4).

Using the proof of Lemma 4.3, there exists a constant C such that

$$\sum_{\sigma_{KL} \in \mathcal{E}_T} |\lambda_{KL}^T| (\psi_K^n - \psi_L^n)^2 \le C m_T,$$

where m_T denotes the measure of the triangle T. Therefore, (6.2) implies that

$$0 \leq P_m \leq C \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{T \in \mathcal{T}_m} m_T \mu \left(\bar{\phi}_T^{n+1} - \underline{\phi}_T^{n+1} \right)^2$$

$$\leq C \iint_{\Omega_T} \mu \left(\bar{\phi}_{\mathcal{T}_m, \Delta t_m} - \underline{\phi}_{\mathcal{T}_m, \Delta t_m} \right)^2 dx dt.$$

Since μ is bounded, continuous with $\mu(0) = 0$, it is enough to show that up to an unlabeled subsequence $\bar{\phi}_{\mathcal{T}_m,\Delta t_m} - \underline{\phi}_{\mathcal{T}_m,\Delta t_m} \to 0$ a.e. in Ω_T in order to conclude the proof of $\lim_{m\to\infty} P_m = 0$. By a generalization of Lemma A.1 in [13], there holds

$$\iint_{\Omega_T} \left| \bar{\phi}_{\mathcal{T}_m, \Delta t_m}(t, x) - \underline{\phi}_{\mathcal{T}_m, \Delta t_m}(t, x) \right|^2 dx dt \le C h_m^2 \|\nabla \phi(v)_{\mathcal{T}_m, \Delta t_m}\|_{L^2(\Omega_T)}^2.$$

Consequently, by Lemma 4.2, ellipticity of Λ and Lemma 4.5, one obtains

$$\iint_{\Omega_T} \left| \bar{\phi}_{\mathcal{T}_m, \Delta t_m}(t, x) - \underline{\phi}_{\mathcal{T}_m, \Delta t_m}(t, x) \right|^2 \! dx dt \leq C h_m^2.$$

Hence, up to a subsequence,

$$\lim_{m \to \infty} D_{1,m} = \lim_{m \to \infty} P_m = 0.$$

Now, we prove that

$$\lim_{m \to \infty} D_{2,m} = \iint_{\Omega_T} \Lambda \nabla v \cdot \nabla \psi dx dt.$$

For this sake, we introduce the term $D_{2,m}^*$ defined by:

$$D_{2,m}^* := \iint_{\Omega_T} \Theta_{\mathcal{T}_m, \Delta t_m} \Lambda(x) \nabla \phi(v)_{\mathcal{T}_m, \Delta t_m} \cdot \nabla \psi_{\mathcal{T}_m, \Delta t_m} (\cdot, t - \Delta t_m) dx dt,$$

where $\Theta_{\mathcal{T}_m,\Delta t_m}$ is a piecewise constant (per triangle) function given by

$$\Theta_{\mathcal{T}_m,\Delta t_m}(t,x) = \sqrt{\eta \circ \phi^{-1}} \Big(\Phi_{\mathcal{T}_m,\Delta t_m}(t,x) \Big), \quad \forall x \in T, t \in (t_n, t_{n+1}], \forall T \in \mathcal{T}_m,$$

and

$$\Phi_{\mathcal{T}_m,\Delta t_m}(t,x) = \phi(v)_{\mathcal{T}_m,\Delta t_m}(t,x_T), \quad \forall x \in T, t \in (t_n,t_{n+1}], \forall T \in \mathcal{T}_m,$$

where x_T is the center of mass of T. Adapting a slightly modified version of the proof of Lemma A.1 in [13], it is simple to check that

$$\Phi_{\mathcal{T}_m,\Delta t_m} \to \phi(v) \text{ in } L^2(\Omega_T) \text{ as } m \to \infty.$$

Moreover, the function $\sqrt{\eta \circ \phi^{-1}}$ being continuous and bounded, one gets

$$\Theta_{\mathcal{T}_m,\Delta t_m} \to \sqrt{\eta(v)} \text{ in } L^2(\Omega_T) \text{ as } m \to \infty.$$

Furthermore, $\nabla \phi(v)_{\mathcal{T}_m, \Delta t_m}$ converges weakly in $L^2(\Omega_T)$ to $\nabla \phi(v)$ and $\nabla \psi_{\mathcal{T}_m, \Delta t_m}$ converges uniformly to $\nabla \psi$. Hence,

$$\lim_{m \to \infty} D_{2,m}^* = \iint_{\Omega_T} \sqrt{\eta(v)} \Lambda(x) \nabla \phi(v) \cdot \nabla \psi dx dt$$
$$= \iint_{\Omega_T} \Lambda(x) \nabla v \cdot \nabla \psi dx dt,$$

where the last equality follows from the observation that

$$\nabla \phi(v) = \frac{1}{\sqrt{\eta(v)}} \nabla v.$$

Therefore, it is only required to verify that

$$|D_{2,m} - D_{2,m}^*| \to 0 \text{ as } m \to \infty.$$

Introducing the notation

$$\eta_T^{n+1} := \left(\Theta_{\mathcal{T}_m, \Delta t_m}(t_{n+1}, x_T)\right)^2, \quad \forall \ T \in \mathcal{T}_m, \forall \ n \in \{0, \dots, N_m - 1\},$$

then the discrete form of $D_{2,m}^*$ becomes

$$D_{2,m}^* = \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{T \in \mathcal{T}_m} \sqrt{\eta_T^{n+1}} \sum_{\sigma_{KL} \in \mathcal{E}_T} \lambda_{KL}^T \Big(\phi(v_K^{n+1}) - \phi(v_L^{n+1}) \Big) (\psi_K^n - \psi_L^n).$$

By a similar argument to the one used in getting inequality (6.1), there holds

$$\left| \sqrt{\eta_{KL}^{n+1}} - \sqrt{\eta_T^{n+1}} \right| \le \mu \left(\bar{\phi}_T^{n+1} - \underline{\phi}_T^{n+1} \right), \quad \forall \ \sigma_{KL} \in \mathcal{E}_T.$$

Therefore,

$$|D_{2,m} - D_{2,m}^*|^2 \leq \Bigg(\sum_{n=0}^{N_m-1} \Delta t_m \sum_{T \in \mathcal{T}_m} \mu \Big(\bar{\phi}_T^{n+1} - \underline{\phi}_T^{n+1}\Big) \sum_{\sigma_{KL} \in \mathcal{E}_T} |\lambda_{KL}^T| |\phi(v_K^{n+1}) - \phi(v_L^{n+1})| |\psi_K^n - \psi_L^n| \Bigg)^2.$$

Using Cauchy-Schwarz' inequality, we get

$$|D_{2,m} - D_{2,m}^*|^2 \leq \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{T \in \mathcal{T}_m} \mu \Big(\bar{\phi}_T^{n+1} - \underline{\phi}_T^{n+1} \Big)^2 \sum_{\sigma_{KL} \in \mathcal{E}_T} |\lambda_{KL}^T| (\psi_K^n - \psi_L^n)^2 \times \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{T \in \mathcal{T}_m} \sum_{\sigma_{KL} \in \mathcal{E}_T} |\lambda_{KL}^T| |\phi(v_K^{n+1}) - \phi(v_L^{n+1})|^2,$$

Using Lemmata 4.2, 4.3 and 4.5, there exists C independent of h_m such that

$$|D_{2,m} - D_{2,m}^*|^2 \le C \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{T \in \mathcal{T}_m} \mu \Big(\bar{\phi}_T^{n+1} - \underline{\phi}_T^{n+1} \Big)^2 \sum_{\sigma_{KL} \in \mathcal{E}_T} |\lambda_{KL}^T| (\psi_K^n - \psi_L^n)^2 := Q_m,$$

and the same argument as in the proof of $\lim_{m\to\infty} P_m = 0$, implies that $\lim_{m\to\infty} Q_m = 0$. Hence,

$$\lim_{m \to \infty} |D_{2,m} - D_{2,m}^*| = 0.$$

Reaction term

It is required to prove now that

$$\lim_{m \to \infty} R_m = -\iint_{\Omega_T} I_{\text{ion}}(v(t, x), \mathbf{w}(t, x), c(t, x)) \psi(t, x) dx dt := R.$$

First rewrite R_m and R as:

$$R_m = -\sum_{n=0}^{N_m - 1} \sum_{K \in \mathcal{V}} \int_{t_n}^{t_{n+1}} \int_{\omega_K} I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \psi(t_n, x_K),$$

and

$$R = \sum_{n=0}^{N_m - 1} \sum_{K \in \mathcal{V}} \int_{t_n}^{t_{n+1}} \int_{\omega_K} -I_{\text{ion}}(v, \mathbf{w}, c) \psi(t, x) dx dt.$$

Then note that $|R_m - R|$ can be written as:

$$\begin{split} |R_m - R| &= \Big| \sum_{n=0}^{N_m - 1} \sum_{K \in \mathcal{V}_m} \Bigg[I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \int_{t_n}^{t_{n+1}} \int_{\omega_K} \Big(\psi(t_n, x_K) - \psi(t, x) \Big) \\ &+ \int_{t_n}^{t_{n+1}} \int_{\omega_K} \Big(I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n) \psi(t, x) - I_{\text{ion}}(v, \mathbf{w}, c) \psi(t, x) \Big) \Bigg] \Big|. \end{split}$$

For all $x \in \omega_K$ and $t \in [t_n, t_{n+1}]$, there holds

$$|\psi(t_n, x_K) - \psi(t, x)| \le C_1(\Delta t_m + h_m),$$

for some $C_1 > 0$. Moreover, $|\psi(t,x)| \leq C_2$ for some $C_2 > 0$. Therefore,

$$|R_m - R| \leq C_1(\Delta t_m + h_m) \sum_{n=0}^{N_m - 1} \Delta t_m \sum_{K \in \mathcal{V}_m} m_K |I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n)|$$

$$+ C_2 \iint_{\Omega_T} |I_{\text{ion}}(v_{\mathcal{M}_m, \Delta t_m}, \mathbf{w}_{\mathcal{M}_m, \Delta t_m}, c_{\mathcal{M}_m, \Delta t_m}) - I_{\text{ion}}(v, \mathbf{w}, c)| dx dt.$$

Since $|I_{\text{ion}}(v_K^{n+1}, \mathbf{w}_K^{n+1}, c_K^n)|$ is bounded, we get

$$|R_m - R| \le C_3(\Delta t_m + h_m)T|\Omega| + C_2 \iint_{\Omega_T} |I_{\text{ion}}(v_{\mathcal{M}_m, \Delta t_m}, \mathbf{w}_{\mathcal{M}_m, \Delta t_m}, c_{\mathcal{M}_m, \Delta t_m}) - I_{\text{ion}}(v, \mathbf{w}, c)| dx dt.$$

On the other hand, since $v_{\mathcal{M}_m,\Delta t_m} \to v$, $\mathbf{w}_{\mathcal{M}_m,\Delta t_m} \to \mathbf{w}$, and $c_{\mathcal{M}_m,\Delta t_m} \to c$ a.e. in Ω_T and I_{ion} is continuous, then $I_{\text{ion}}(v_{\mathcal{M}_m,\Delta t_m},\mathbf{w}_{\mathcal{M}_m,\Delta t_m},c_{\mathcal{M}_m,\Delta t_m}) \to I_{\text{ion}}(v,\mathbf{w},c)$ a.e. in Ω_T . Moreover, since $I_{\text{ion}}(v_{\mathcal{M}_m,\Delta t_m},\mathbf{w}_{\mathcal{M}_m,\Delta t_m},c_{\mathcal{M}_m,\Delta t_m}) \in L^{\infty}(\Omega_T)$, then by Lebesgue's dominated convergence we get the convergence of $I_{\text{ion}}(v_{\mathcal{M}_m,\Delta t_m},\mathbf{w}_{\mathcal{M}_m,\Delta t_m},\mathbf{w}_{\mathcal{M}_m,\Delta t_m},c_{\mathcal{M}_m,\Delta t_m})$ to $I_{\text{ion}}(v,\mathbf{w},c)$ in $L^1(\Omega_T)$. As a result, we conclude that $R_m \to R$.

This ends the proof of convergence of discrete solutions to the weak solution.

7. Numerical Results

In this section, we illustrate the efficiency of the nonlinear CVFE scheme (3.12), (3.6), (3.7) and we compare it to the CVFE scheme (3.5), (3.6), (3.7). Newton's algorithm is used to solve the nonlinear systems. For our test, we consider a rectangular domain permitting to visualize all the phases of the action potential (fast depolarization, short repolarization period, plateau, repolarization). We fix: $\Delta t = 0.5$, $\chi = 1000$, $C_m = 1$.

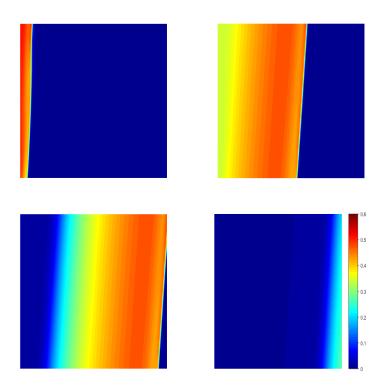


FIGURE 2. From up left to down right consecutively: The propagation of the action potential for t=10, 200, 350, 600 ms respectively using CVFE scheme.

We assume that the conductivity tensor is anisotropic and is given by:

$$\Lambda = \left(\begin{array}{cc} 1.2042 & 0.4500 \\ 0.4500 & 0.1843 \end{array}\right),$$

which eigenvalues are $\lambda_1 = 0.0141$ and $\lambda_2 = 1.3744$. Due to the anisotropy condition, a vertical stimulus at the left side of the domain propagates in a slanted way towards the right side of the domain in both schemes, see Figures 2 and 3. As expected from the previous analysis, the maximum principle is verified in the case of the positive nonlinear CVFE scheme (3.12), (3.6), (3.7). In particular, the values of the rescaled potential difference v are between 0 and 1. However,

in the CVFE scheme (3.5), (3.6), (3.7), it takes negative values corresponding to unphysiological ones. This is clearly seen in the fluctuation below -85 mV observed in the graph of the action potential in Figure 4. In the same figure, the results of a finite element simulation (implemented with freefem++) using the same conditions is shown. One can easily observe the oscillations in the wave (drawn in 3D) obtained by both the FE scheme and the CVFE scheme. Such oscillations are absent when the positive CVFE scheme is used.

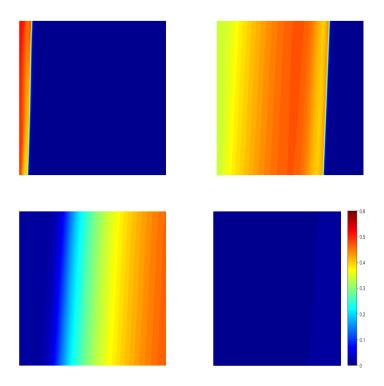


FIGURE 3. From up left to down right consecutively: The propagation of the action potential for t=10, 200, 350, 600 ms respectively using the positive nonlinear CVFE scheme.

Furthermore, we have tested the positive CVFE scheme on a 2D-domain imitating a cross section of the heart with the left and right ventricles. The mesh is shown in Figure 5. We initiated a stimulus in the interventricular septal wall, and we recorded the propagation of the action potential using two different conductivities:

$$\Lambda_1 = \left(\begin{array}{cc} 1.2042 & 0 \\ 0 & 0.1843 \end{array} \right) \text{ and } \Lambda_2 = \left(\begin{array}{cc} 1.2042 & 0.4500 \\ 0.4500 & 0.1843 \end{array} \right).$$

Figures 6 and 8 show the propagation of the electrical wave in the 2D section for the diagonal and the full conductivity matrices Λ_1 and Λ_2 respectively. The propagation of the wave is clearly different. On the other hand, the recorded action potential at the points A, B, C, D and E indicated in Figure 5 are very close to the physiological Action Potential of Beeler-Reuter model especially in points D and E as shown in Figures 7 and 9.

8. Conclusion

In conclusion, we have studied, in this work, a positive nonlinear CVFE scheme for the monodomain model coupled with Beeler-Reuter ionic model. The aim was to approximate the fluxes properly keeping in mind that the solutions must satisfy some natural bounds in addition to some estimates on the discrete gradients. The numerical tests exhibited the ability of the nonlinear

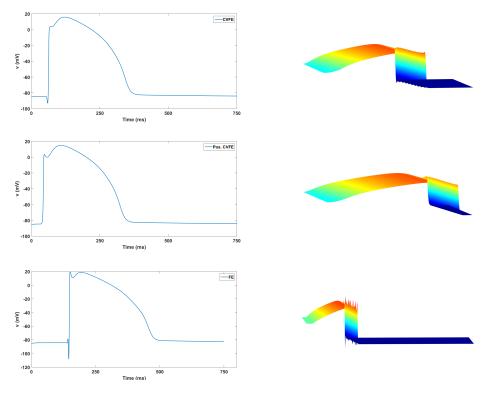


FIGURE 4. First Column: Action potentials obtained from the CVFE scheme (top), the positive nonlinear CVFE scheme (center) and the finite elements method (bottom) at the same point. Second column: the respective wave propagation at time $t=250~\rm ms$.

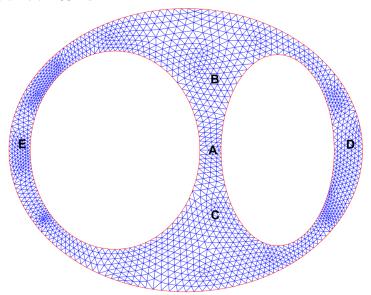


FIGURE 5. The mesh of the cross section and the points at which the action potential is drawn.

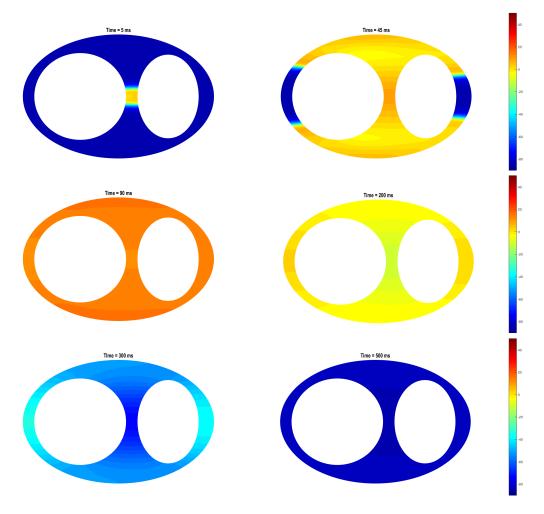


FIGURE 6. The propagation of the action potential using the conductivity Λ_1 at t = 10, 45, 90, 200, 300 and 500 ms from top left to bottom right respectively.

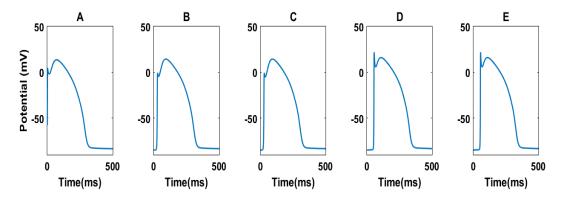


FIGURE 7. Action potentials recorded at the points A, B, C, D and E using conductivity Λ_1 .

CVFE scheme to efficiently simulate the propagation of the action potential without any overand undershoots. However, some numerical diffusion is observed during the simulations mainly due to the upwind technique.

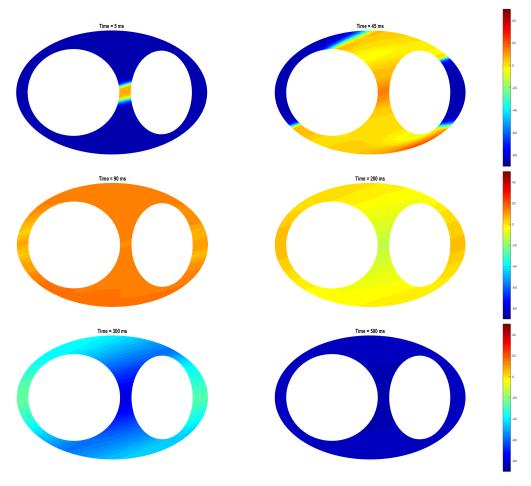


FIGURE 8. The propagation of the action potential using the conductivity Λ_2 at t = 10, 45, 90, 200, 300 and 500 ms from top left to bottom right respectively.

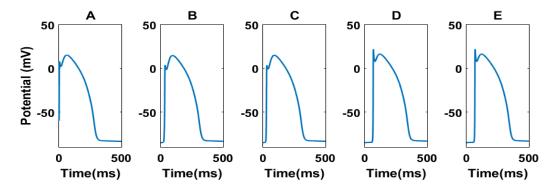


FIGURE 9. Action potentials recorded at the points A, B, C, D and E using conductivity Λ_2 .

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