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An Approximation of Three-Dimensional Semiconductor Devices by Mixed Finite Element Method and Characteristics-Mixed Finite Element Method

Qing Yang[1,*], Yirang Yuan[2]

[1]*School of Mathematical Science, Shandong Normal University, Jinan, 250014, China.*
[2]*Institute of Mathematics, Shandong University, Jinan, 250100, China.*

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Abstract. The mathematical model for semiconductor devices in three space dimensions are numerically discretized. The system consists of three quasi-linear partial differential equations about three physical variables: the electrostatic potential, the electron concentration and the hole concentration. We use standard mixed finite element method to approximate the elliptic electrostatic potential equation. For the two convection-dominated concentration equations, a characteristics-mixed finite element method is presented. The scheme is locally conservative. The optimal L^2-norm error estimates are derived by the aid of a post-processing step. Finally, numerical experiments are presented to validate the theoretical analysis.

AMS subject classifications: 65M15; 65M60

Key words: Three-dimensional semiconductor devices, characteristics-mixed finite element method, mixed finite element method, post-processing step, error bound.

1. Introduction

The numerical simulation of the transient behavior of semiconductor devices is of great value both in theory and in practice (cf. [6, 17]). The production of actual semiconductor devices is mainly based on a planar technology. However, the down-scaling of the devices brings some severe problems such as increase of power densities and noise effects. The use of multi-gate field-effect transistors is a possible solution to reduce the noise. In such devices, the gate contact encloses the channel region from different sides to lead to smaller no-signal currents. But such devices require to be modeled and numerically simulated in three space dimensions. In this paper, we will consider the drift-diffusion model of three-dimensional semiconductor devices. The

*Corresponding author. *Email address:* sd_yangq@163.com (Q. Yang); yryuan@sdu.edu.cn (Y. Yuan)

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mathematical model is a coupled system of three quasi-linear partial differential equations with initial and boundary conditions (cf. [2, 4, 12, 18, 19]). The equation for the electrostatic potential is a Poisson equation. The continuity equations for the electrons and holes are of convection-dominated diffusion type. The model is described by the following system

$$-\Delta\psi = \nabla \cdot u = \alpha(p - e + F(x)), \qquad (x,t) \in \Omega \times [0,T], \tag{1.1a}$$

$$\frac{\partial e}{\partial t} = \nabla \cdot [D_e(x)\nabla e + \mu_e(x)eu] - R(e,p), \qquad (x,t) \in \Omega \times J, \tag{1.1b}$$

$$\frac{\partial p}{\partial t} = \nabla \cdot [D_p(x)\nabla p - \mu_p(x)pu] - R(e,p), \qquad (x,t) \in \Omega \times J, \tag{1.1c}$$

where $J = (0,T]$, and Ω is a bounded domain in $\mathcal{R}^3$. Here ψ, e and p are the electrostatic potential, the electron and hole concentrations, respectively. $u = -\nabla\psi$ is the electric field. $\alpha = q/\vartheta$, where $q > 0$ is the electronic charge and $\vartheta > 0$ is the dielectric permittivity. $D_s(x)(s = e, p)$ are the diffusion coefficients which are related to the carrier mobilities $\mu_s(x)(s = e, p)$ through the Einstein relation $D_s(x) = U_T\mu_s(x)$, with U_T being the thermal voltage. $R(e,p)$ is the net recombination rate. $F(x) = N_D(x) - N_A(x)$ is the doping profile in the device, where $N_D(x)$ and $N_A(x)$ are the donor and acceptor impurity concentrations, respectively.

We consider the following boundary and initial conditions

$$-\left.\frac{\partial\psi}{\partial\nu}\right|_{\partial\Omega} = u \cdot \nu = 0, \qquad \left.\frac{\partial e}{\partial\nu}\right|_{\partial\Omega} = 0, \qquad \left.\frac{\partial p}{\partial\nu}\right|_{\partial\Omega} = 0, \quad t \in J, \tag{1.1d}$$

$$e(x,0) = e_0(x),\ p(x,0) = p_0(x), \quad x \in \Omega, \tag{1.1e}$$

where ν is the unit outward normal vector on boundary $\partial\Omega$.

The following compatibility condition (cf. [17])

$$\int_\Omega (p_0 - e_0 + F)dx = 0 \tag{1.1f}$$

must be imposed on the data in order that a solution is possible. In addition, we apply the conditions

$$\int_\Omega \psi dx = 0,\ 0 \le t \le T \tag{1.1g}$$

to determine a unique ψ for each t.

In reality (1.1b) and (1.1c) might be strongly convection-dominated when $D_s(s = e, p)$ are quite small. In such circumstance, the standard Galerkin or difference scheme does not work well any more. In order to obtain better approximations, a variety of numerical techniques, such as characteristic finite element method (cf. [18]), characteristic finite difference method (cf. [4, 19]), upwind finite volume method (cf. [14–16]), etc., have been used for (1.1) in two or three space dimensions.

Although the modified method of characteristic finite element method (MMOC-Galerkin) (cf. [5, 9]) has advantages of avoidance of numerical diffusion and nonphysical oscillations and smaller time-truncation, it fails to preserve local mass balance. Preserving mass locally is of great importance in practice. In [1], Arbogast and Wheeler

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proposed a characteristics-mixed method for approximating an advection-dominated transport problem. The scheme, which was based on a space-time variational form, used a characteristic approximation to handle advection in time and a lowest-order mixed finite element spatial approximation to discretize the diffusion term. Mass was conserved element by element because piecewise constants were in the space of test functions. In order to improve the rate of convergence of the method, a post-processing step was included in the scheme. However, the scheme included many integrals of the test function's mappings which were very difficult to be evaluated and used in practical computation.

In [13], Sun and Yuan defined a combined approximation scheme for the two-dimensional incompressible miscible displacement in porous media. It used standard mixed finite element for the Darcy velocity equation and a characteristics-mixed finite element method for the concentration equation. Characteristic approximation was applied to handle the hyperbolic part of the concentration equation, and a lowest-order mixed finite element spatial approximation was employed to treat the diffusion term. Although the scheme was much easier to compute compared to that in [1], only global conservation of mass was proved for it.

In this paper, we will propose a combined numerical method for the system (1.1). Note that it is the electric field intensity u but not the electrostatic potential ψ that appears explicitly in (1.1b) and (1.1c). Consequently, we choose standard mixed finite element method for the electrostatic potential equation. The electrostatic potential and the electric field intensity are approximated simultaneously. The direct approximation of the electric field intensity will give improved approximate accuracy of the concentrations for the same computational effort. A characteristics-mixed finite element method which preserve mass locally is presented for approximating the electron and hole concentrations. That is, the hyperbolic parts of the two concentration equations are approximated along characteristics, and the diffusion terms are approximated by using lowest-order mixed finite element method. The scheme of this combined numerical method is locally conservative. We conduct the convergence analysis of the scheme and obtain optimal L^2-norm error estimates by the aid of a post-processing step. Finally, we present some numerical experiments to validate the theoretical analysis.

In this paper, we use the following notations and norms of Sobolev spaces:

$$L^2(\Omega) = \left\{ f : \int_\Omega |f|^2 dx < \infty \right\}, \quad \|f\| = \left[\int_\Omega |f|^2 dx \right]^{1/2},$$
$$L^\infty(\Omega) = \{ f : \operatorname{ess}\sup_\Omega |f| < \infty \}, \quad \|f\|_{L^\infty} = \operatorname{ess}\sup_\Omega |f|,$$

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and for $m \geq 0$,

$$H^m(\Omega) = \left\{ f : \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \in L^2(\Omega), |\alpha| \leq m \right\}, \qquad \|f\|_m = \left[\sum_{|\alpha| \leq m} \left\| \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \right\|^2 \right]^{1/2},$$

$$W_\infty^m(\Omega) = \left\{ f : \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \in L^\infty(\Omega), |\alpha| \leq m \right\}, \qquad \|f\|_{W_\infty^m} = \max_{|\alpha| \leq m} \left\| \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \right\|_{L^\infty}.$$

In particular, $H^0(\Omega) = L^2(\Omega)$, $W_\infty^0(\Omega) = L^\infty(\Omega)$. Let $[a, b] \subset [0, T]$ and X be a Sobolev space. For any function $f(x, t)$ defined on $\Omega \times [a, b]$, we set for $m \geq 0$,

$$H^m(a, b; X) = \left\{ f : \int_a^b \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X^2 dt < \infty, \alpha \leq m \right\},$$

$$\|f\|_{H^m(a,b;X)} = \left[\sum_{\alpha=0}^m \int_a^b \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X^2 dt \right]^{1/2},$$

$$W_\infty^m(a, b; X) = \left\{ f : \operatorname{ess\,sup}_{[a,b]} \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X < \infty, \alpha \leq m \right\},$$

$$\|f\|_{W_\infty^m(a,b;X)} = \max_{0 \leq \alpha \leq m} \operatorname{ess\,sup}_{[a,b]} \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X,$$

$$L^2(a, b; X) = H^0(a, b; X), \quad L^\infty(a, b; X) = W_\infty^0(a, b; X).$$

For convenience, we drop $[a, b] = [0, T]$ and Ω from the notations. For example, we write $L^2(H^1)$ for $L^2(0, T; H^1(\Omega))$.

For a vector function $v = (v_1, v_2, v_3)$, we say that $v \in X^3$ if $v_i \in X$ $(i = 1, 2, 3)$. We also define the following spaces of vector-functions and norms

$$H^m(\text{div}; \Omega) = \left\{ v : v_1, v_2, v_3, \nabla \cdot v \in H^m(\Omega) \right\},$$

$$\|v\|_{H^m(\text{div})} = [\|v_1\|_m^2 + \|v_2\|_m^2 + \|v_3\|_m^2 + \|\nabla \cdot v\|_m^2]^{1/2}, \quad m \geq 0,$$

$$H(\text{div}; \Omega) = H^0(\text{div}; \Omega).$$

We use the following assumptions on the regularity of the solutions of (1.1)

$$(\mathtt{R}) \quad \begin{cases} e, p \in L^\infty(H^2) \cap H^1(H^1) \cap L^\infty(W_\infty^1) \cap H^2(L^2), \\ \psi \in L^\infty(H^1), \\ u \in L^\infty(H^1(\text{div})) \cap L^\infty((W_\infty^1)^3) \cap W_\infty^1((L^\infty)^2) \cap H^2((L^2)^3). \end{cases}$$

We make explicit use of the following tacit conditions on the coefficients in (1.1)

$$(\mathtt{C}) \quad 0 \leq D_* \leq D_s(x) \leq D^*, \quad |\mu_s(x)| + |\nabla \mu_s(x)| \leq \mu^*, \quad s = e, p,$$

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here D_*, D^* and μ^* are positive constants. From [6], we know that these assumptions are reasonable in physics. We assume that $R(e,p)$ is Lipschitz continuous in some ε_0-neighborhood of the solutions. Exactly, there exist positive constants ε_0 and K, such that for any $|\varepsilon_i| \le \varepsilon_0$ $(i=1,2)$,

$$\begin{aligned}&|R(e(x,t),p(x,t)) - R(e(x,t)+\varepsilon_1, p(x,t)+\varepsilon_2)|\\ \le& K\Big(|\varepsilon_1|+|\varepsilon_2|\Big), \quad (x,t)\in\Omega\times[0,T].\end{aligned} \tag{1.2}$$

An outline of this paper is as follows. In Section 2, we first formulate the characteristics-mixed finite element method for the concentration equations and mixed finite element method for the electrostatic potential equation, respectively. Then we define the combined approximation scheme by combining the characteristics-mixed finite element and mixed finite element method. A post-processing step is introduced to aid the convergence analysis. We list some properties of finite element spaces and projections in Section 3. The optimal-order error estimates are derived in Section 4. Finally in Section 5, we conduct some numerical experiments to validate our theoretical conclusion.

Throughout, we will use the symbols K and ε to denote a generic positive constant and a generic small positive constant, respectively, which may have different values at different occurrences.

2. Formulation of the methods

2.1. A characteristics-mixed method for the concentrations

In this subsection, we assume that an electric field intensity $u=(u_1,u_2,u_3)$ from (1.1a) is given and concentrate on defining the locally conservative characteristics-mixed method for (1.1b) (also for (1.1c)). Noticing the insulated condition (1.1d), which can be treated as a reflection boundary, it is reasonable to assume that Ω is a cuboid and that (1.1) is Ω-periodic. Throughout the rest of this paper, we assume that all functions are spatially Ω-periodic. Thus, we can drop the boundary condition (1.1d).

Define

$$V=\Big\{\chi:\chi\in H(\mathrm{div};\Omega),\ \chi\cdot\nu|_{\partial\Omega}=0\Big\},$$

$$\mathcal{M}=\Big\{\varphi:\varphi\in L^2(\Omega),\varphi\ \texttt{is piecewise constant}\Big\};\quad \mathcal{M}\ \texttt{is dense in}\ L^2(\Omega).$$

Denote by $\tau_e(x,t)$ and $\tau_p(x,t)$ the unit vectors in the directions of $(-\mu_e u_1,-\mu_e u_2,-\mu_e u_3,1)$ and $(\mu_p u_1,\mu_p u_2,\mu_p u_3,1)$, respectively. Thus, we can write

$$\phi_e\frac{\partial e}{\partial\tau_e}=\frac{\partial e}{\partial t}-\mu_e u\cdot\nabla e,\qquad \phi_p\frac{\partial p}{\partial\tau_p}=\frac{\partial p}{\partial t}+\mu_p u\cdot\nabla p,$$

where

$$\phi_s=\Big(\mu_s^2|u|^2+1\Big)^{1/2}=\Big(\mu_s^2(u_1^2+u_2^2+u_3^2)+1\Big)^{1/2},\quad s=e,p.$$

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Let $z_e = -D_e\nabla e$ and $z_p = -D_p\nabla p$. The weak form of (1.1b) and (1.1c) is the problem of finding a map $(e, z_e, p, z_p) : [0,T] \to L^2(\Omega) \times V \times L^2(\Omega) \times V$, such that

$$\left(\phi_e \frac{\partial e}{\partial \tau_e}, \varphi\right) + (\nabla \cdot z_e, \varphi) - (e\nabla \cdot (\mu_e u), \varphi)$$
$$= -(R(e,p), \varphi), \qquad \forall \varphi \in L^2(\Omega), \tag{2.1a}$$

$$(D_e^{-1} z_e, \chi) - (e, \nabla \cdot \chi) = 0, \qquad \forall \chi \in V, \tag{2.1b}$$

$$\left(\phi_p \frac{\partial p}{\partial \tau_p}, \varphi\right) + (\nabla \cdot z_p, \varphi) + (p\nabla \cdot (\mu_p u), \varphi) = -(R(e,p), \varphi),$$
$$\forall \varphi \in L^2(\Omega), \tag{2.1c}$$

$$(D_p^{-1} z_p, \chi) - (p, \nabla \cdot \chi) = 0, \qquad \forall \chi \in V, \tag{2.1d}$$

$$e(x,0) = e_0(x), \quad p(x,0) = p_0(x), \quad z_e(x,0) = -D_e(x)\nabla e_0(x),$$
$$z_p(x,0) = -D_p(x)\nabla p_0(x), \qquad \forall x \in \Omega. \tag{2.1e}$$

Partition $[0,T]$ into $0 = t^0 < t^1 < \cdots < t^N$, with $\Delta t_c^n = t^n - t^{n-1}$. For convenience, we drop the superscript from Δt_c^n, but we point out that our analysis is still valid for variable time steps. For functions f defined on $\Omega \times [0,T]$, we write $f^n(x)$ for $f(x,t^n)$. Define

$$\bar{x}_e^{n-1} = x + \mu_e u^n \Delta t_c, \qquad \bar{e}^{n-1}(x) = e^{n-1}(\bar{x}_e^{n-1});$$
$$\bar{x}_p^{n-1} = x - \mu_p u^n \Delta t_c, \qquad \bar{p}^{n-1}(x) = p^{n-1}(\bar{x}_p^{n-1}).$$

Applying the backward difference quotient in the τ_e-direction to approximate $(\partial e^n/\partial \tau_e)(x) = (\partial e/\partial \tau_e)(x, t^n)$, we get

$$\frac{\partial e^n}{\partial \tau_e}(x) \approx \frac{e^n(x) - \bar{e}^{n-1}(x)}{\Delta t_c \phi_e^n}.$$

Similarly, we have

$$\frac{\partial p^n}{\partial \tau_p}(x) \approx \frac{p^n(x) - \bar{p}^{n-1}(x)}{\Delta t_c \phi_p^n}.$$

Thus, we have immediately

$$\phi_e^n \frac{\partial e^n}{\partial \tau_e} \approx \frac{e^n(x) - \bar{e}^{n-1}(x)}{\Delta t_c}, \qquad \phi_p^n \frac{\partial p^n}{\partial \tau_p} \approx \frac{p^n(x) - \bar{p}^{n-1}(x)}{\Delta t_c}. \tag{2.2}$$

In order to discretize (2.1) in the space variables, we define a family of quasi-uniform regular meshes $\mathcal{T}_{h_c}$ of Ω with diameter of each element bounded by h_c. Let $M_h \times H_h \in \mathcal{M} \times V$ be the lowest-order Raviart-Thomas-Nédélec mixed finite element spaces (cf. [7, 8]).

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Combining the time difference (2.2) with the standard mixed finite element method in the space variables, we define the characteristics-mixed approximation of the weak form (2.1) as follows: for any $n \geq 0$, find $(e_h^n, p_h^n, z_{eh}^n, z_{ph}^n) \in M_h \times M_h \times H_h \times H_h$ such that

$$\left(\frac{e_h^n - \bar{e}_h^{n-1}}{\Delta t_c}, \varphi\right) + (\nabla \cdot z_{eh}^n, \varphi) - (e_h^{n-1} \nabla \cdot (\mu_e u^n), \varphi)$$
$$= -(R(e_h^{n-1}, p_h^{n-1}), \varphi), \quad \forall \varphi \in M_h, \tag{2.3a}$$
$$(D_e^{-1} z_{eh}^n, \chi) - (e_h^n, \nabla \cdot \chi) = 0, \quad \forall \chi \in H_h, \tag{2.3b}$$
$$\left(\frac{p_h^n - \bar{p}_h^{n-1}}{\Delta t_c}, \varphi\right) + (\nabla \cdot z_{ph}^n, \varphi) + (p_h^{n-1} \nabla \cdot (\mu_p u^n), \varphi)$$
$$= -(R(e_h^{n-1}, p_h^{n-1}), \varphi), \quad \forall \varphi \in M_h, \tag{2.3c}$$
$$(D_p^{-1} z_{ph}^n, \chi) - (p_h^n, \nabla \cdot \chi) = 0, \quad \forall \chi \in H_h, \tag{2.3d}$$
$$e_h^0 = \tilde{e}_h^0, \quad p_h^0 = \tilde{p}_h^0, \quad z_{eh}^0 = \tilde{z}_e^0, \quad z_{ph}^0 = \tilde{z}_p^0, \quad \forall x \in \Omega, \tag{2.3e}$$

where $(\tilde{e}_h, \tilde{p}_h, \tilde{z}_e, \tilde{z}_p)$ are elliptic projections of (e, p, z_e, z_p) into $M_h \times M_h \times H_h \times H_h$, which will be defined in next section.

2.2. A mixed FEM for the electrostatic potential and electric field intensity

Let

$$W = L^2(\Omega) \setminus \{w \equiv \texttt{constant on } \Omega\}.$$

Write (1.1a) as

$$u = -\nabla \psi, \qquad x \in \Omega,\ t \in [0, T], \tag{2.4a}$$
$$\nabla \cdot u = \alpha(p - e + F), \qquad x \in \Omega,\ t \in [0, T]. \tag{2.4b}$$

The family of saddle-point problems of (2.4) is given by a map $(u, \psi) : [0, T] \to V \times W$ satisfying

$$(u, v) - (\psi, \nabla \cdot v) = 0, \qquad \forall v \in V, \tag{2.5a}$$
$$(\nabla \cdot u, w) = \alpha(p - e + F, w), \qquad \forall w \in W. \tag{2.5b}$$

For any $h_\psi > 0$, let $\mathcal{T}_{h_\psi}$ be a quasi-uniform regular mesh of Ω with diameter of each element bounded by h_ψ and $V_h \times W_h \in V \times W$ be Raviart-Thomas-Nédélec spaces of index $k = 0$ defined on this mesh (cf. [7, 8]). Given concentration approximations e_h and p_h at $t \in [0, T]$, the mixed finite element method for approximating the electrostatic potential and the electric field intensity reads as finding $(u_h(\cdot, t), \psi_h(\cdot, t)) \in V_h \times W_h$ such that

$$(u_h, v) + (\psi_h, \nabla \cdot v) = 0, \qquad \forall v \in V_h, \tag{2.6a}$$
$$(\nabla \cdot u_h, w) = \alpha(p_h - e_h + F, w), \qquad \forall w \in W_h. \tag{2.6b}$$

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2.3. The combined approximation scheme

In practice, the electric field intensity usually changes less rapidly in time than the electron and hole concentrations. Thus, it is appropriate to use longer time steps for (2.6) than for (2.3). We partition $[0,T]$ into electrostatic potential time steps $0=t_0<t_1<\cdots<t_M=T$ and let $\Delta t_\psi^m=t_m-t_{m-1}$. In general, $\Delta t_\psi^m>\Delta t_c$. We may use variable Δt_ψ^m, but we drop the superscript except for Δt_ψ^1. We set each electrostatic potential level to be also a concentration level, i.e., for each m there exists n such that $t_m=t^n$. Let $j=\Delta t_\psi/\Delta t_c$ and $j_1=\Delta t_\psi^1/\Delta t_c$. For functions $f(x,t)$, we use the notation $f_m(x)=f(x,t_m)$. Thus, subscripts correspond to electrostatic potential levels and superscripts to concentration levels.

For each $n\geq 1$, if the concentration level t^n relates to potential levels by $t_{m-1}<t^n\leq t_m$, we shall use an electric field intensity approximation Eu_h^n to replace u^n in (2.3a) and (2.3c). If $m\geq 2$, set

$$Eu_h^n=\left(1+\frac{t^n-t_{m-1}}{t_{m-1}-t_{m-2}}\right)u_{h,m-1}-\frac{t^n-t_{m-1}}{t_{m-1}-t_{m-2}}u_{h,m-2};$$

if $m=1$, set

$$Eu_h^n=u_{h0}.$$

We notice that Eu_h^n is first-order in time during the first electrostatic potential level and second-order during later levels. It explains why we have retained the superscript of Δt_ψ^1.

By combining (2.3) and (2.6), we now define our time-stepping numerical procedure for solving (1.1), which finds $(e_h,z_{eh},p_h,z_{ph}):\{t^0,t^1,\cdots,t^N\}\to M_h\times H_h\times M_h\times H_h$ and $(u_h,\psi_h):\{t_0,t_1,\cdots,t_M\}\to V_h\times W_h$ such that

$$\left(\frac{e_h^n-\hat{e}_h^{n-1}}{\Delta t_c},\varphi\right)+(\nabla\cdot z_{eh}^n,\varphi)-(e_h^{n-1}\nabla\cdot(\mu_e Eu_h^n),\varphi)$$
$$=-(R(e_h^{n-1},p_h^{n-1}),\varphi),\qquad \forall\varphi\in M_h,\quad n\geq 1, \tag{2.7a}$$

$$(D_e^{-1}z_{eh}^n,\chi)-(e_h^n,\nabla\cdot\chi)=0,\qquad \forall\chi\in H_h,\quad n\geq 1, \tag{2.7b}$$

$$\left(\frac{p_h^n-\hat{p}_h^{n-1}}{\Delta t_c},\varphi\right)+(\nabla\cdot z_{ph}^n,\varphi)+(p_h^{n-1}\nabla\cdot(\mu_p Eu_h^n),\varphi)$$
$$=-(R(e_h^{n-1},p_h^{n-1})),\varphi),\qquad \forall\varphi\in M_h,\quad n\geq 1, \tag{2.7c}$$

$$(D_p^{-1}z_{ph}^n,\chi)-(p_h^n,\nabla\cdot\chi)=0,\qquad \forall\chi\in H_h,\quad n\geq 1, \tag{2.7d}$$

$$e_h^0=\tilde{e}_h^0,\quad p_h^0=\tilde{p}_h^0,\quad z_{eh}^0=\tilde{z}_e^0,\quad z_{ph}^0=\tilde{z}_p^0,\qquad \forall x\in\Omega, \tag{2.7e}$$

$$(u_{hm},v)+(\psi_{hm},\nabla\cdot v)=0,\qquad \forall v\in V_h,\quad m\geq 0, \tag{2.7f}$$

$$(\nabla\cdot u_{hm},w)=\alpha(p_{hm}-e_{hm}+F,w),\qquad \forall w\in W_h,\quad m\geq 0, \tag{2.7g}$$

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where

$$\hat{e}_h^{n-1}(x) = e_h^{n-1}(\hat{x}_e^{n-1}) = e_h^{n-1}\left(x + \mu_e E u_h^n \Delta t_c\right),$$
$$\hat{p}_h^{n-1}(x) = p_h^{n-1}(\hat{x}_p^{n-1}) = p_h^{n-1}\left(x - \mu_p E u_h^n \Delta t_c\right).$$

The numerical procedure (2.7) is computed in the order as follows:

- (1) compute $(e_h^0, z_{eh}^0, p_h^0, z_{ph}^0)$ from initial data, then solve (u_{h0}, ψ_{h0}) from (2.7f) and (2.7g);
- (2) solve $(e_h^1, z_{eh}^1, p_h^1, z_{ph}^1)$, $\cdots$, $(e_h^{j_1}, z_{eh}^{j_1}, p_h^{j_1}, z_{ph}^{j_1})$ from (2.7a)$\sim$ (2.7d);
- (3) noting that $(e_h^{j_1}, p_h^{j_1}) = (e_{h1}, p_{h1})$, calculate (u_{h1}, ψ_{h1}) from (2.7f) and (2.7);
- (4) calculate $(e_h^{j_1+1}, z_{eh}^{j_1+1}, p_h^{j_1+1}, z_{ph}^{j_1+1})$, $\cdots$, $(e_h^{j_1+j}, z_{eh}^{j_1+j}, p_h^{j_1+j}, z_{ph}^{j_1+j})$, (u_{h2}, ψ_{h2}) in similar order;
- (5) calculate the approximations in turn analogically at other time levels.

Let $\mathcal{M}_h$ be a space of discontinuous and piecewise linear functions over the mesh $\mathcal{T}_{h_c}$. We begin by finding some appropriate approximations $(E_h^0, P_h^0) \in \mathcal{M}_h \times \mathcal{M}_h$ to (e_0, p_0). For each $n \geq 1$ and each $m \geq 0$, we find first $(e_h^n, z_{eh}^n, p_h^n, z_{ph}^n) \in M_h \times H_h \times M_h \times H_h$ and $(u_{hm}, \psi_{hm}) \in V_h \times W_h$ such that

$$\left(\frac{e_h^n - \hat{E}_h^{n-1}}{\Delta t_c}, \varphi\right) + (\nabla \cdot z_{eh}^n, \varphi) - (E_h^{n-1} \nabla \cdot (\mu_e E u_h^n), \varphi)$$
$$= -(R(\hat{E}_h^{n-1}, \hat{P}_h^{n-1}), \varphi), \qquad \forall \varphi \in M_h, \quad n \geq 1, \tag{2.8a}$$
$$(D_e^{-1} z_{eh}^n, \chi) - (e_h^n, \nabla \cdot \chi) = 0, \qquad \forall \chi \in H_h, \quad n \geq 1, \tag{2.8b}$$
$$\left(\frac{p_h^n - \hat{P}_h^{n-1}}{\Delta t_c}, \varphi\right) + (\nabla \cdot z_{ph}^n, \varphi) + (P_h^{n-1} \nabla \cdot (\mu_p E u_h^n), \varphi)$$
$$= -(R(\hat{E}_h^{n-1}, \hat{P}_h^{n-1})), \varphi), \qquad \forall \varphi \in M_h, \quad n \geq 1, \tag{2.8c}$$
$$(D_p^{-1} z_{ph}^n, \chi) - (p_h^n, \nabla \cdot \chi) = 0, \qquad \forall \chi \in H_h, \quad n \geq 1, \tag{2.8d}$$
$$(u_{hm}, v) + (\psi_{hm}, \nabla \cdot v) = 0, \qquad \forall v \in V_h, \quad m \geq 0, \tag{2.8e}$$
$$(\nabla \cdot u_{hm}, w) = \alpha(P_{hm} - E_{hm} + F, w), \qquad \forall w \in W_h, \quad m \geq 0. \tag{2.8f}$$

We then locally postprocess (e_h^n, p_h^n) by defining $(E_h^n, P_h^n) \in \mathcal{M}_h \times \mathcal{M}_h$ such that

$$(E_h^n - e_h^n, 1)_{\mathcal{B}} = 0, \tag{2.9a}$$
$$(D_e \nabla E_h^n + z_{eh}^n, \nabla \omega)_{\mathcal{B}} = 0, \qquad \forall \omega \in \mathcal{M}_h, \tag{2.9b}$$
$$(P_h^n - p_h^n, 1)_{\mathcal{B}} = 0, \tag{2.9c}$$
$$(D_p \nabla P_h^n + z_{ph}^n, \nabla \omega)_{\mathcal{B}} = 0, \qquad \forall \omega \in \mathcal{M}_h, \tag{2.9d}$$

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for any element $\mathcal{B} \in \mathcal{T}_{h_c}$.

The steps of computation are as follows:

- (1) when (E_h^0, P_h^0) are given, solve (u_{h0}, ψ_{h0}) by (2.8e) and (2.8f);
- (2) use (2.8a)$\sim$(2.8d) to solve $(e_h^1, z_{eh}^1, p_h^1, z_{ph}^1)$, then use post-processing step (2.9) to obtain (E_h^1, P_h^1);
- (3) analogically, for $1 \le n \le j_1$, when $(e_h^{n-1}, z_{eh}^{n-1}, p_h^{n-1}, z_{ph}^{n-1})$ are known, use (2.9) to obtain (E_h^{n-1}, P_h^{n-1}), then use (2.8a)$\sim$(2.8d) to solve $(e_h^n, z_{eh}^n, p_h^n, z_{ph}^n)$ and use (2.9) to compute (E_h^n, P_h^n);
- (4) noting that $(E_h^{j_1}, P_h^{j_1}) = (E_{h1}, P_{h1})$, then use (2.8e) and (2.8f) to solve (u_{h1}, ψ_{h1});
- (5) similarly, calculate in turn $(e_h^{j_1+1}, z_{eh}^{j_1+1}, p_h^{j_1+1}, z_{ph}^{j_1+1})$, (E^{j_1+1}, P^{j_1+1}), $\cdots$, $(e_h^{j_1+j}, z_{eh}^{j_1+j}, p_h^{j_1+j}, z_{ph}^{j_1+j})$, $(E_h^{j_1+j}, P_h^{j_1+j}) = (E_{h2}, P_{h2})$, (u_{h2}, ψ_{h2});
- (6) calculate approximations at other time levels step by step as above.

2.4. Principle of local mass conservation

Assume that the recombination rate $R(e,p) = 0$ and the boundary insulates, we can derive the following principle of local mass conservation on each $\mathcal{B} \in \mathcal{T}_{h_c}$,

$$\int_{\mathcal{B}} \frac{\partial e}{\partial t} dx + \int_{\partial \mathcal{B}} z_e \cdot \nu_{\mathcal{B}} ds - \int_{\partial \mathcal{B}} \mu_e(x) eu \cdot \nu_{\mathcal{B}} ds = 0,$$
$$\int_{\mathcal{B}} \frac{\partial p}{\partial t} dx + \int_{\partial \mathcal{B}} z_p \cdot \nu_{\mathcal{B}} ds + \int_{\partial \mathcal{B}} \mu_p(x) pu \cdot \nu_{\mathcal{B}} ds = 0.$$

We now turn to prove that the corresponding discrete principle of local mass conservation holds.

Theorem 2.1. *Assuming $R(e,p) = 0$, then on each $\mathcal{B} \in \mathcal{T}_{h_c}$, we have*

$$\int_{\mathcal{B}} \frac{e_h^n - \hat{e}_h^{n-1}}{\Delta t_c} dx + \int_{\partial \mathcal{B}} z_{eh}^n \cdot \nu_{\mathcal{B}} ds - \int_{\partial \mathcal{B}} \mu_e e_h^{n-1} E u_h^n \cdot \nu_{\mathcal{B}} ds = 0, \tag{2.10}$$
$$\int_{\mathcal{B}} \frac{p_h^n - \hat{p}_h^{n-1}}{\Delta t_c} dx + \int_{\partial \mathcal{B}} z_{ph}^n \cdot \nu_{\mathcal{B}} ds + \int_{\partial \mathcal{B}} \mu_p p_h^{n-1} E u_h^n \cdot \nu_{\mathcal{B}} ds = 0. \tag{2.11}$$

Proof. For each element $\mathcal{B} \in \mathcal{T}_{h_c}$, by choosing φ in (2.7a) to be the characteristic function on $\mathcal{B}$, we get

$$\int_{\mathcal{B}} \frac{e_h^n - \hat{e}_h^{n-1}}{\Delta t_c} dx + \int_{\mathcal{B}} \nabla \cdot z_{eh}^n dx - \int_{\mathcal{B}} e_h^{n-1} \nabla \cdot (\mu_e E u_h^n) dx = 0.$$

Since $e_h^{n-1} \in M_h$ is a constant on $\mathcal{B}$ and the normal component of $u_{hm} \in V_h$ continues across interior element boundaries over the mesh $\mathcal{T}_{h_\psi}$, (2.10) follows from the use of integration by parts to the second and third left-hand side terms.

The result (2.11) can be proved from (2.7c) by a completely similar argument. □

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3. Properties of finite element spaces and some projections

3.1. For the concentrations

From [7,8], the spaces $H_h \times M_h$ and $\mathcal{M}_h$ satisfy the following approximation and inverse properties

$$(\mathtt{A}_c)\quad \begin{cases} \inf\limits_{\varphi\in M_h} \|f-\varphi\| \le K_0 h_c \|f\|_1, \\ \inf\limits_{\chi\in H_h} \|g-\chi\| \le K_0 h_c \|g\|_1, \\ \inf\limits_{\chi\in H_h} \|g-\chi\|_{H(\mathrm{div})} \le K_0 h_c \|g\|_{H^1(\mathrm{div})}, \end{cases}$$

$$(\mathtt{I}_c)\quad \begin{cases} \|\varphi\|_{L^\infty} \le K_0 h_c^{-3/2} \|\varphi\|, \quad \forall \varphi \in M_h, \\ \|\omega\|_{L^\infty} \le K_0 h_c^{-3/2} \|\omega\|, \quad \forall \omega \in \mathcal{M}_h. \end{cases}$$

For each $t \in [0,T]$, we define the projections $(\tilde{e}_h, \tilde{z}_e, \tilde{p}_h, \tilde{z}_p) \in M_h \times H_h \times M_h \times H_h$ of the exact solutions (e, z_e, p, z_p), such that

$$(\tilde{s}_h - s, \varphi) + (\nabla\cdot(\tilde{z}_s - z_s), \varphi) = 0, \qquad \forall \varphi \in M_h, \quad s = e, p, \tag{3.1a}$$

$$(D_s^{-1}(\tilde{z}_s - z_s), \chi) + (\tilde{s}_h - s, \nabla\cdot\chi) = 0, \qquad \forall \chi \in H_h, \quad s = e, p. \tag{3.1b}$$

We can get the existence and uniqueness of $(\tilde{s}_h, \tilde{z}_s)$ from [7,8].

Using $(\tilde{z}_e, \tilde{z}_p)$, we can post-process $(\tilde{e}_h, \tilde{p}_h)$ to obtain $(\tilde{E}_h, \tilde{P}_h)$. $\tilde{E}_h \in \mathcal{M}_h$ is defined by

$$(\tilde{E}_h - \tilde{e}_h, 1)_{\mathcal{B}} = 0, \tag{3.2a}$$

$$(D_e \nabla \tilde{E}_h + \tilde{z}_e, \nabla\omega)_{\mathcal{B}} = 0, \qquad \forall \omega \in \mathcal{M}_h. \tag{3.2b}$$

Similarly, $\tilde{P}_h$ can also be defined. Denote

$$\eta_e = \tilde{e}_h - e, \quad \xi_e = e_h - \tilde{e}_h; \quad \tilde{\eta}_e = \tilde{E}_h - e, \quad \tilde{\xi}_e = E_h - \tilde{E}_h;$$
$$\rho_e = \tilde{z}_e - z_e, \quad \zeta_e = z_{eh} - \tilde{z}_e,$$

η_p, ξ_p, and so on, are similar.

The counterparts of following Lemmas can be found in [1] or [8].

Lemma 3.1. (cf. [1,8]) *For any $t \in [0,T]$ and $h_c > 0$ sufficiently small,*

$$\|\eta_s\| \le K_1 h_c \|z_s\|_1, \quad \|\rho_s\| \le K_1 h_c \|z_s\|_1, \tag{3.3a}$$

$$\|\tilde{\eta}_s\| \le K_1 \Big(\|z_s\|_1 + \|\nabla\cdot z_s\|_1 \Big) h_c^2, \tag{3.3b}$$

$$\left\| \frac{\partial \tilde{\eta}_s}{\partial t} \right\| \le K_1 \left(\|z_s\|_1 + \|\nabla\cdot z_s\|_1 + \left\| \frac{\partial z_s}{\partial t} \right\|_1 + \left\| \nabla\cdot \frac{\partial z_s}{\partial t} \right\|_1 \right) h_c^2, \tag{3.3c}$$

$$\left(\sum_{\mathcal{B}\in\mathcal{T}_{h_c}} \|\nabla\tilde{\eta}_s\|_{\mathcal{B}}^2 \right)^{1/2} \le K_1 \|z_s\|_1 h_c, \tag{3.3d}$$

where $s = e, p$.

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By the inverse inequality (I_c) and a priori estimation (3.3c), there exists a constant $K_2 > 0$ independent of h_c such that

$$\|\tilde{E}_h\|_{L^\infty(L^\infty)} \le K_2, \qquad \|\tilde{P}_h\|_{L^\infty(L^\infty)} \le K_2. \tag{3.4}$$

Lemma 3.2. (cf. [1]) *We have*

$$(\tilde{\xi}_s^n - \xi_s^n, \tilde{\xi}_s^n) = \|\tilde{\xi}_s^n - \xi_s^n\|^2, \tag{3.5a}$$
$$\|\xi_s^n\| \le \|\tilde{\xi}_s^n\|, \tag{3.5b}$$
$$\|D_s^{1/2}\nabla\tilde{\xi}_s^n\|_{\mathcal{B}} \le \|D_s^{-1/2}\zeta_s^n\|_{\mathcal{B}}, \tag{3.5c}$$
$$\|\tilde{\xi}_s^n - \xi_s^n\|_{\mathcal{B}} \le K_3\|\nabla\tilde{\xi}_s^n\|_{\mathcal{B}}h_c, \tag{3.5d}$$

where $s = e, p$ and K_3 is a positive constant independent of h_c.

Lemma 3.3. (cf. [1]) *For each positive integer n, there exist functions $\Phi_s^n \in H^1(\Omega)$, $s = e, p$, such that*

$$\|\Phi_s^n\|_1 \le \{\|\xi_s^n\|_{-1} + \|\zeta_s^n\|\}, \quad s = e, p,$$

and, for sufficiently small h_c,

$$\|\Phi_s^n - \xi_s^n\| \le K_4\Big(\|\xi_s^n\|_{-1} + \|\zeta_s^n\|\Big)h_c, \quad s = e, p,$$

where K_4 depends on the positive upper and lower bounds for D_s and on $\|D_s\|_{W_\infty^1(\Omega)}$, and $\|\cdot\|_{-1}$ denotes the norm of the dual to $H^1(\Omega)$.

Remark 3.1. From the proof of Lemma 6 in (cf. [1]), we know that Φ_s^n $(s = e, p)$ are in the standard Galerkin space of continuous, piecewise linear or trilinear functions (as appropriate) which are defined by their nodal values over the grid $\mathcal{T}_{h_c}$.

3.2. For the electrostatic potential and electric field intensity

The Raviart-Thomas-Nédélec mixed finite element spaces $V_h \times W_h$ have the following properties (cf. [7, 8])

$$(\mathtt{A}_\psi)\quad \begin{cases} \inf\limits_{v\in V_h} \|f - v\| \le K_5 h_\psi \|f\|_1, \\ \inf\limits_{v\in V_h} \|f - v\|_{H(\mathrm{div})} \le K_5 h_\psi \|f\|_{H^1(\mathrm{div})}, \\ \inf\limits_{w\in W_h} \|g - w\| \le K_5 h_\psi \|g\|_1, \end{cases}$$

$$(\mathtt{I}_\psi)\quad \begin{cases} \|v\|_{L^\infty} \le K_5 h_\psi^{-3/2}\|v\|, & \forall v \in V_h, \\ \|v\|_{W_\infty^1(\mathcal{K})} \le K_5 h_\psi^{-1}\|v\|_{L^\infty(\mathcal{K})}, & \forall v \in V_h, \end{cases}$$

where $\mathcal{K}$ is any element in $\mathcal{T}_{h_\psi}$ and K_5 is a positive constant independent of h_ψ.

We introduce a map $(\tilde{u}_h, \tilde{\psi}_h) : [0, T] \to V_h \times W_h$ defined by

$$(\tilde{u}_h, v) - (\tilde{\psi}_h, \nabla \cdot v) = 0, \qquad \forall v \in V_h, \tag{3.6a}$$
$$(\nabla \cdot \tilde{u}_h, w) = (\alpha(p - e + F), w), \qquad \forall w \in W_h. \tag{3.6b}$$

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From [7, 8], $(\tilde{u}_h, \tilde{\psi}_h)$ exists uniquely, and there exists a positive constant K_6 independent of h_ψ, such that

$$\begin{aligned}&\|u-\tilde{u}_h\|_{L^\infty(H(\mathrm{div}))}+\|\psi-\tilde{\psi}_h\|_{L^\infty(L^2)}\\&\le K_6\Big(\|u\|_{L^\infty(H(\mathrm{div}))},\|\psi\|_{L^\infty(H^1)}\Big)h_\psi.\end{aligned}\tag{3.7}$$

From (2.8e), (2.8f) and (3.7), there exists a positive constant K_7 independent of h_ψ, such that

$$\begin{aligned}&\|u_{hm}-\tilde{u}_{hm}\|_{H(\mathrm{div})}+\|\psi_{hm}-\tilde{\psi}_{hm}\|\\&\le K_7\Big(\|e_m-E_{hm}\|+\|p_m-P_{hm}\|\Big)\\&\le K_7\Big(\|\tilde{\eta}_{em}\|+\|\tilde{\eta}_{pm}\|+\|\tilde{\xi}_{em}\|+\|\tilde{\xi}_{pm}\|\Big).\end{aligned}\tag{3.8}$$

4. A priori error estimates

In this Section, we obtain the optimal a priori error estimates. For the approximations of the concentrations and their flux, we have the following optimal convergence rates.

Theorem 4.1. *Suppose that (R), (C), (A_c), (I_c), (A_ψ) and (I_ψ) hold, and that the discretization parameters satisfy the relations*

$$\Delta t_c=O(h_\psi),\ \ h_\psi=O(h_c^{3/2}),\ \ (\Delta t_\psi^1)^{3/2}=O(h_\psi),\ \ (\Delta t_\psi)^2=O(h_\psi).\tag{4.1}$$

If we choose $E_h^0=\tilde{E}_h^0$, $P_h^0=\tilde{P}_h^0$ and if there is a constant K' such that $\Delta t_c\ge K'h_c^{3/2}$, then for h_c and Δt_c sufficiently small,

$$\begin{aligned}&\max_{1\le n\le N}\{\|E_h^n-e^n\|+\|P_h^n-p^n\|\}\\&\le K\Big(h_c^{3/2}+h_\psi+\Delta t_c+(\Delta t_\psi)^2+(\Delta t_\psi^1)^{3/2}\Big),\end{aligned}\tag{4.2}$$

$$\begin{aligned}&\max_{1\le n\le N}\{\|e_h^n-e^n\|+\|p_h^n-p^n\|\}\\&\le K\Big(h_c+h_\psi+\Delta t_c+(\Delta t_\psi)^2+(\Delta t_\psi^1)^{3/2}\Big),\end{aligned}\tag{4.3}$$

$$\begin{aligned}&\left(\sum_{n=1}^N\|z_e^n-z_{eh}^n\|^2\Delta t_c\right)^{1/2}+\left(\sum_{n=1}^N\|z_p^n-z_{ph}^n\|^2\Delta t_c\right)^{1/2}\\&\qquad\le K\{h_c+h_\psi+\Delta t_c+(\Delta t_\psi)^2+(\Delta t_\psi^1)^{3/2}\},\end{aligned}\tag{4.4}$$

where the positive constant K principally depends on (R), (C), (A_c), (I_c), (A_ψ), (I_ψ), (3.3), $\|\partial^2 e/\partial\check{\tau}_e^2\|$ and $\|\partial^2 p/\partial\check{\tau}_p^2\|$, but is independent of Δt_c, Δt_ψ, h_c and h_ψ.

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Proof. From (2.1a), (2.1b) and (3.1), we have

$$\left(\frac{e^n-\hat{e}^{n-1}}{\Delta t_c},\varphi\right)+(\nabla\cdot\tilde{z}_e^n,\varphi)-(e^n\nabla\cdot(\mu_e u^n),\varphi)=-(R(e^n,p^n),\varphi)$$
$$-\left(\phi_e\frac{\partial e^n}{\partial\tau_e}-\frac{e^n-\hat{e}^{n-1}}{\Delta t_c},\varphi\right)-(\eta_e^n,\varphi),\qquad\forall\varphi\in M_h,\tag{4.5a}$$
$$(D_e^{-1}\tilde{z}_e^n,\chi)-(\tilde{e}_h^n,\nabla\cdot\chi)=0,\qquad\forall\chi\in H_h.\tag{4.5b}$$

Combining (2.8a), (2.8b) and (4.5), we get the following error equations

$$\left(\frac{\xi_e^n-\hat{\tilde{\xi}}_e^{n-1}}{\Delta t_c},\varphi\right)+(\nabla\cdot\zeta_e^n,\varphi)$$
$$=(R(e^n,p^n)-R(E_h^{n-1},P_h^{n-1}),\varphi)+\left(\phi_e\frac{\partial e^n}{\partial\tau_e}-\frac{e^n-\hat{e}^{n-1}}{\Delta t_c},\varphi\right)-(e^n\nabla\cdot(\mu_e u^n)$$
$$-E_h^{n-1}\nabla\cdot(\mu_e E u_h^n),\varphi)+(\eta_e^n,\varphi)-\left(\frac{\eta_e^n-\hat{\tilde{\eta}}_e^{n-1}}{\Delta t_c},\varphi\right),\quad\forall\varphi\in M_h,\tag{4.6a}$$
$$(D_e^{-1}\zeta_e^n,\chi)-(\xi_e^n,\nabla\cdot\chi)=0,\quad\forall\chi\in H_h.\tag{4.6b}$$

Choosing the test functions $\varphi=\xi_e^n$ and $\chi=\zeta_e^n$ in (4.6) and then adding (4.6a) and (4.6b) together, we get

$$\left(\frac{\xi_e^n-\hat{\tilde{\xi}}_e^{n-1}}{\Delta t_c},\xi_e^n\right)+(D_e^{-1}\zeta_e^n,\zeta_e^n)$$
$$=(R(e^n,p^n)-R(E_h^{n-1},P_h^{n-1}),\xi_e^n)+\left(\phi_e\frac{\partial e^n}{\partial\tau_e}-\frac{e^n-\hat{e}^{n-1}}{\Delta t_c},\xi_e^n\right)$$
$$-(e^n\nabla\cdot(\mu_e u^n)-E_h^{n-1}\nabla\cdot(\mu_e E u_h^n),\xi_e^n)+(\eta_e^n,\xi_e^n)-\left(\frac{\eta_e^n-\hat{\tilde{\eta}}_e^{n-1}}{\Delta t_c},\xi_e^n\right).\tag{4.7}$$

Combining (3.2a) and (2.9a) yields

$$(\xi_e^n,\varphi)=(\tilde{\xi}_e^n,\varphi),\quad(\eta_e^n,\varphi)=(\tilde{\eta}_e^n,\varphi),\quad\forall\varphi\in M_h.\tag{4.8}$$

Set

$$\check{x}_e^{n-1}=x+\mu_e E u^n\Delta t_c,\qquad\check{f}^{n-1}(x)=f^{n-1}(\check{x}_e^{n-1}),$$

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where f is any function defined on $\Omega \times [0,T]$. Applying (4.8) in (4.7), we have

$$\begin{aligned}
&\left(\frac{\tilde{\xi}_e^n - \tilde{\xi}_e^{n-1}}{\Delta t_c}, \xi_e^n\right) + (D_e^{-1}\zeta_e^n, \zeta_e^n) \\
=&\left(\left[\frac{\partial e^n}{\partial t} - \mu_e E u^n \cdot \nabla e^n\right] - \frac{e^n - \check{e}^{n-1}}{\Delta t_c}, \xi_e^n\right) + (\mu_e[Eu^n - u^n]\cdot\nabla e^n, \xi_e^n) \\
&- (e^n \nabla\cdot(\mu_e u^n) - E_h^{n-1}\nabla\cdot(\mu_e E u_h^n), \xi_e^n) \\
&+ (\tilde{\eta}_e^n, \xi_e^n) + (R(e^n, p^n) - R(E_h^{n-1}, P_h^{n-1}), \xi_e^n) \\
&- \left(\frac{\tilde{\eta}_e^n - \tilde{\eta}_e^{n-1}}{\Delta t_c}, \xi_e^n\right) + \left(\frac{\hat{e}^{n-1} - \check{e}^{n-1}}{\Delta t_c}, \xi_e^n\right) - \left(\frac{\check{\tilde{\eta}}_e^{n-1} - \hat{\tilde{\eta}}_e^{n-1}}{\Delta t_c}, \xi_e^n\right) \\
&- \left(\frac{\check{\tilde{\xi}}_e^{n-1} - \hat{\tilde{\xi}}_e^{n-1}}{\Delta t_c}, \xi_e^n\right) - \left(\frac{\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}}{\Delta t_c}, \xi_e^n\right) - \left(\frac{\tilde{\xi}_e^{n-1} - \check{\tilde{\xi}}_e^{n-1}}{\Delta t_c}, \xi_e^n\right). \qquad (4.9)
\end{aligned}$$

For the first term on the left-hand side of (4.9), it follows from Holder's inequality and (4.8) that

$$\begin{aligned}
(\tilde{\xi}_e^n - \tilde{\xi}_e^{n-1}, \xi_e^n) \geq& (\tilde{\xi}_e^n, \xi_e^n) - \frac{1}{2}[(\tilde{\xi}_e^{n-1}, \tilde{\xi}_e^{n-1}) + (\xi_e^n, \xi_e^n)] \\
=& \frac{1}{2}(\tilde{\xi}_e^n, \xi_e^n) - \frac{1}{2}(\tilde{\xi}_e^{n-1}, \tilde{\xi}_e^{n-1}) \\
=& \frac{1}{2}\left[(\tilde{\xi}_e^n, \tilde{\xi}_e^n) - (\tilde{\xi}_e^{n-1}, \tilde{\xi}_e^{n-1})\right] - \frac{1}{2}(\tilde{\xi}_e^n - \xi_e^n, \tilde{\xi}_e^n).
\end{aligned}$$

Using Lemma 3.2, we have

$$(\tilde{\xi}_e^n - \xi_e^n, \tilde{\xi}_e^n) = \|\tilde{\xi}_e^n - \xi_e^n\|^2 \leq K_3 \sum_{\mathcal{B}\in\mathcal{T}_{h_c}} \|\nabla\tilde{\xi}_e^n\|_{\mathcal{B}}^2 h_c^2 \leq K_3' h_c^2 \|D_e^{-1/2}\zeta_e^n\|^2.$$

Thus, we bound the left-hand side of (4.9) as follows

$$\begin{aligned}
&\frac{1}{\Delta t_c}(\tilde{\xi}_e^n - \tilde{\xi}_e^{n-1}, \xi_e^n) + (D_e^{-1}\zeta_e^n, \zeta_e^n) \\
\geq& \frac{1}{2\Delta t_c}\left[(\tilde{\xi}_e^n, \tilde{\xi}_e^n) - (\tilde{\xi}_e^{n-1}, \tilde{\xi}_e^{n-1})\right] + \frac{1}{2\Delta t_c}(2\Delta t_c - K_3' h_c^2)(D_e^{-1}\zeta_e^n, \zeta_e^n). \qquad (4.10)
\end{aligned}$$

We denote the right-hand side terms of (4.9) by $T_1, T_2, \cdots, T_{11}$ and estimate these terms one by one.

In order to estimate T_1, we write

$$\frac{\partial e^n}{\partial t} - \mu_e E u^n \cdot \nabla e^n = \sigma \frac{\partial e^n}{\partial \check{\tau}_e}, \quad \sigma(x) = [1 + \mu_e^2 |Eu^n|^2]^{1/2},$$

where $\check{\tau}_e$ is the unit vector along $(-\mu_e E u^n, 1)$. From [5, 9], we obtain

$$|T_1| \leq K \left\| \frac{\partial^2 e}{\partial \check{\tau}_e^2} \right\|_{L^2(t^{n-1}, t^n; L^2)}^2 \Delta t_c + K\|\xi_e^n\|^2. \qquad (4.11)$$

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For T_2, we see that

$$\begin{aligned}|T_2| \leq & \|\mu_e \nabla e^n\|_{L^\infty} \|u^n - Eu^n\| \|\xi_e^n\| \\ \leq & K(\Delta t_\psi)^3 \left\| \frac{\partial^2 u}{\partial t^2} \right\|^2_{L^2(t_{m-2}, t_m; L^2)} + K\|\xi_e^n\|^2. \end{aligned} \tag{4.12}$$

When $t^n \leq t_1$, the temporal error term should be replaced by $K(\Delta t_\psi^1)^2 \|\partial u/\partial t\|^2_{L^2(t_0,t_1;L^2)}$.

For the estimate of T_3, we write

$$\begin{aligned}|T_3| = & |(e^n \nabla \cdot (\mu_e u^n) - E_h^{n-1} \nabla \cdot (\mu_e E u_h^n), \xi_e^n)| \\ \leq & |(e^n \nabla \cdot (\mu_e u^n) - E_h^{n-1} \nabla \cdot (\mu_e u^n), \xi_e^n)| \\ & + |(\tilde{E}_h^{n-1} \nabla \cdot (\mu_e u^n) - E_h^{n-1} \nabla \cdot (\mu_e E u_h^n), \xi_e^n)| \\ & + |(\tilde{\xi}_e^{n-1} \nabla \cdot (\mu_e u^n) - E_h^{n-1} \nabla \cdot (\mu_e E u_h^n), \Phi_e^n)| \\ & + |(\tilde{\xi}_e^{n-1} \nabla \cdot (\mu_e u^n) - E_h^{n-1} \nabla \cdot (\mu_e E u_h^n), \xi_e^n - \Phi_e^n)|. \end{aligned}$$

Noting the remark about Φ_e^n after Lemma 3.3, we have the following inequality as in [10]

$$\|\Phi_e^n\|_{L^\infty} \leq K h_c^{-1/2} \|\Phi_e^n\|_1.$$

Then, the above inequality, the Lemma 3.3 and the inverse property (I_c) give that

$$\begin{aligned}|T_3| \leq & \Big(\|e^n - E_h^{n-1}\| \|\nabla \cdot (\mu_e u^n)\|_{L^\infty} + \|\tilde{E}_h^{n-1}\|_{L^\infty} \|\nabla \cdot [\mu_e (u^n - Eu_h^n)]\| \Big) \|\xi_e^n\| \\ & + \|\tilde{\xi}_e^{n-1}\| \|\nabla \cdot [\mu_e (u^n - Eu_h^n)]\| \|\Phi_e^n\|_{L^\infty} + \|\tilde{\xi}_e^{n-1}\|_{L^\infty} \|\nabla \cdot [\mu_e (u^n - Eu_h^n)]\| \|\xi_e^n - \Phi_e^n\| \\ \leq & K \Big(\|e^n - e^{n-1}\| + \|\tilde{\eta}_e^{n-1}\| + \|\tilde{\xi}_e^{n-1}\| + \|u^n - Eu^n\|_{H(\mathrm{div})} + \|Eu^n - Eu_h^n\|_{H(\mathrm{div})} \Big) \|\xi_e^n\| \\ & + K h_c^{-1/2} \|\tilde{\xi}_e^{n-1}\| \|\nabla \cdot [\mu_e (u^n - Eu_h^n)]\| \|\Phi_e^n\|_1 \\ & + K h_c^{-3/2} \|\tilde{\xi}_e^{n-1}\| \|\nabla \cdot [\mu_e (u^n - Eu_h^n)]\| \|\xi_e^n - \Phi_e^n\| \\ \leq & K \Big(\|e^n - e^{n-1}\| + \|\tilde{\eta}_e^{n-1}\| + \|\tilde{\xi}_e^{n-1}\| + \|u^n - Eu^n\|_{H(\mathrm{div})} + \|Eu^n - Eu_h^n\|_{H(\mathrm{div})} \Big) \|\xi_e^n\| \\ & + K h_c^{-1/2} \|\tilde{\xi}_e^{n-1}\| (\|u^n - Eu^n\|_{H(\mathrm{div})} + \|Eu^n - Eu_h^n\|_{H(\mathrm{div})}) (\|\xi_e^n\|_{-1} + \|\zeta_e^n\|) \\ \leq & K \Big(\|e^n - e^{n-1}\| + \|\tilde{\eta}_e^{n-1}\| + \|\tilde{\xi}_e^{n-1}\| \Big) \|\xi_e^n\| \\ & + K(1 + h_c^{-1/2} \|\tilde{\xi}_e^{n-1}\|) \Big(\|u^n - Eu^n\|_{H(\mathrm{div})} + \|Eu^n - Eu_h^n\|_{H(\mathrm{div})} \Big) \|\xi_e^n\| \\ & + K h_c^{-1/2} \|\tilde{\xi}_e^{n-1}\| \Big(\|u^n - Eu^n\|_{H(\mathrm{div})} + \|Eu^n - Eu_h^n\|_{H(\mathrm{div})} \Big) \|\zeta_e^n\|. \end{aligned}$$

Now we need an induction hypothesis. For any fixed integer $l \geq 1$ such that $t^l \leq T$, assume that

$$h_c^{-1} \|\tilde{\xi}_e^{n-1}\|^2 \to 0, \quad h_c^{-1} \|\tilde{\xi}_p^{n-1}\|^2 \to 0, \quad h_c \to 0, \quad n = 1, \cdots, l. \tag{4.13}$$

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Applying (4.18), (3.7), (3.8) and (3.3c), we have

$$|T_3| \le K\left(\left\|\frac{\partial e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;L^2)}\Delta t_c + h_c^4 + h_\psi^2 + (\Delta t_\psi)^3\left\|\frac{\partial^2 u}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_m;H(\mathrm{div}))}\right)$$
$$+ K\left(\|\tilde{\xi}_e^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\tilde{\xi}_{e,m-1}\|^2 + \|\tilde{\xi}_{e,m-2}\|^2 + \|\tilde{\xi}_{p,m-1}\|^2 + \|\tilde{\xi}_{p,m-2}\|^2\right)$$
$$+ \varepsilon\|D_e^{-1/2}\zeta_e^n\|^2, \tag{4.14}$$

for h_c sufficiently small. The remark after (4.12) about the temporal error term applies here as well.

For T_4, using Holder's inequality and (3.3c), we can easily get

$$|T_4| \le \frac{1}{2}\left(\|\tilde{\eta}_e^n\|^2 + \|\xi_e^n\|^2\right) \le K\left(h_c^4 + \|\xi_e^n\|^2\right). \tag{4.15}$$

By using (1.2), we have

$$\begin{aligned}|T_5| \le& K\left(\|e^n - E_h^{n-1}\| + \|p^n - P_h^{n-1}\|\right)\|\xi_e^n\|\\ \le& K\left(\|e^n - e^{n-1}\| + \|p^n - p^{n-1}\| + \|\tilde{\eta}_e^{n-1}\| + \|\tilde{\xi}_e^{n-1}\| + \|\tilde{\eta}_p^{n-1}\| + \|\tilde{\xi}_p^{n-1}\|\right)\|\xi_e^n\|\\ \le& K\left(\Delta t_c\left\|\frac{\partial e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;L^2)} + \Delta t_c\left\|\frac{\partial p}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;L^2)} + h_c^4\right.\\ &\left. + \|\tilde{\xi}_e^{n-1}\|^2 + \|\tilde{\xi}_p^{n-1}\|^2 + \|\xi_e^n\|^2\right).\end{aligned} \tag{4.16}$$

By (3.3d), we have, for the bound of T_6,

$$\begin{aligned}|T_6| \le& K(\Delta t_c)^{-1}\left\|\frac{\partial\tilde{\eta}_e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;L^2)} + K\|\xi_e^n\|^2\\ \le& K(\Delta t_c)^{-1}h_c^4\left(\|z_e\|^2_{L^2(t^{n-1},t^n;H^1)} + \|\nabla\cdot z_e\|^2_{L^2(t^{n-1},t^n;H^1)}\right.\\ &\left. + \left\|\frac{\partial z_e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;H^1)} + \left\|\nabla\cdot\frac{\partial z_e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;H^1)}\right) + K\|\xi_e^n\|^2.\end{aligned} \tag{4.17}$$

To bound T_7, as in [5.9], we first deduce that

$$\begin{aligned}\hat{e}^{n-1} - \check{e}^{n-1} &= \int_{\check{x}_e^{n-1}}^{\hat{x}_e^{n-1}}\frac{\partial e^{n-1}}{\partial z}dz\\ &= \int_0^1\frac{\partial e^{n-1}}{\partial z}((1-\bar{z})\check{x}_e^{n-1} + \bar{z}\hat{x}_e^{n-1})|\mu_e||Eu^n - Eu_h^n|\Delta t_c d\bar{z},\end{aligned} \tag{4.18}$$

where z denotes the unit vector in the direction of $Eu_h^n - Eu^n$. Define

$$g_e(x) = \int_0^1\frac{\partial e^{n-1}}{\partial z}((1-\bar{z})\check{x}_e^{n-1} + \bar{z}\hat{x}_e^{n-1})d\bar{z}.$$

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Noting that $g_e(x)$ is an average of certain first partial derivatives of e^{n-1}, we have

$$\|g_e\|_{L^\infty} \le K\|e^{n-1}\|_{W^1_\infty}.$$

Thus, (4.18), (3.7), (3.8) and (3.3c) imply that

$$\begin{aligned}
|T_7| &= \left|\int_\Omega g_e(x)|\mu_e||Eu^n - Eu_h^n|\xi_e^n dx\right| \\
&\le \|g_e\|_{L^\infty}\|\mu_e(Eu^n - Eu_h^n)\|\|\xi_e^n\| \le K\Big(\|Eu^n - Eu_h^n\|^2 + \|\xi_e^n\|^2\Big) \\
&\le K\{h_\psi^2 + h_c^4 + \|\tilde{\xi}_{e,m-1}\|^2 + \|\tilde{\xi}_{e,m-2}\|^2 + \|\tilde{\xi}_{p,m-1}\|^2 + \|\tilde{\xi}_{p,m-2}\|^2 + \|\xi_e^n\|^2\}. \qquad (4.19)
\end{aligned}$$

Now, we come to bound T_8. We see that

$$\begin{aligned}
|\hat{x}_e^{n-1} - \check{x}_e^{n-1}| &= |\mu_e E(u^n - u_h^n)\Delta t_c| \\
&\le |\mu_e|\Big(\|Eu^n - E\tilde{u}_h^n\|_{L^\infty} + \|E\tilde{u}_h^n - Eu_h^n\|_{L^\infty}\Big)\Delta t_c.
\end{aligned}$$

From [3, 11], it can be expected that

$$\|Eu^n - E\tilde{u}_h^n\|_{L^\infty} \to 0, \quad h_\psi \to 0.$$

Noting that for $v \in V_h$, $\|v\|_{1,\mathcal{K}} \le \|v\|_{H(\mathrm{div};\mathcal{K})}$, we can obtain

$$\begin{aligned}
\|E\tilde{u}_h^n - Eu_h^n\|_{L^\infty(\mathcal{K})} &\le Kh_\psi^{-1/2}\|E\tilde{u}_h^n - Eu_h^n\|_{1,\mathcal{K}} \\
&\le Kh_\psi^{-1/2}\|E\tilde{u}_h^n - Eu_h^n\|_{H(\mathrm{div};\mathcal{K})}.
\end{aligned}$$

Note that we will prove (inductively) that $\|\tilde{\xi}_{e,m-i}\| = O[h_c^{3/2} + h_\psi + \Delta t_c + (\Delta t_\psi^1 + (\Delta t_\psi^2))]$. This fact, (3.8) and (3.3c) imply that

$$\|E\tilde{u}_h^n - Eu_h^n\|_{L^\infty} \to 0, \quad h_c \to 0.$$

Thus, we conclude that

$$|\hat{x}_e^{n-1} - \check{x}_e^{n-1}| = o(1)\Delta t_c, \quad h_c \to 0.$$

Then, it is reasonable to assume that, for each $x \in \mathcal{B}$, $\hat{x}_e^{n-1}$ and $\check{x}_e^{n-1}$ belong to one element $\mathcal{B}'$, for sufficiently small h_c. Thus, using (4.18), (3.3e), (3.3c), (3.7), Lemma 3.3

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and (3.8), we get the bound

$$
\begin{aligned}
|T_8| &= \left| \sum_{\mathcal{B}\in\mathcal{T}_{h_c}} \int_{\mathcal{B}} \frac{\hat{\tilde{\eta}}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}}{\Delta t_c} \xi_e^n dx \right| = \left| \sum_{\mathcal{B}\in\mathcal{T}_{h_c}} \int_{\mathcal{B}} g_{\eta_e} |\mu_e| |Eu^n - Eu_h^n| \xi_e^n dx \right| \\
&\le K \left(\sum_{\mathcal{B}\in\mathcal{T}_{h_c}} \|g_{\tilde{\eta}_e}\|_{\mathcal{B}}^2 \right)^{1/2} \|Eu^n - Eu_h^n\| (\|\Phi_e^n\|_{L^\infty} + \|\Phi_e^n - \xi_e^n\|_{L^\infty}) \\
&\le K \left(\sum_{\mathcal{B}\in\mathcal{T}_{h_c}} \|\nabla\tilde{\eta}_e^{n-1}\|_{\mathcal{B}}^2 \right)^{1/2} \|Eu^n - Eu_h^n\| h_c^{-1/2} (\|\xi_e^n\|_{-1} + \|\zeta_e^n\|) \\
&\le K \Big(h_\psi^2 + h_c^4 + \|\tilde{\xi}_{e,m-1}\|^2 + \|\tilde{\xi}_{e,m-2}\|^2 + \|\tilde{\xi}_{p,m-1}\|^2 + \|\tilde{\xi}_{p,m-2}\|^2 + \|\xi_e^n\|^2 \Big) \\
&\quad + \varepsilon \|D_e^{-1/2} \zeta_e^n\|^2. \qquad (4.20)
\end{aligned}
$$

Handling T_9 in the manner as T_8, we obtain

$$
\begin{aligned}
|T_9| &\le K \left(\sum_{\mathcal{B}\in\mathcal{T}_h} \|\nabla\tilde{\xi}_e^{n-1}\|_{\mathcal{B}}^2 \right)^{1/2} \|Eu^n - Eu_h^n\| h_c^{-1/2} \Big(\|\xi_e^n\|_{-1} + \|\zeta_e^n\| \Big) \\
&\le K \|D_e^{-1/2} \zeta_e^{n-1}\| h_c^{-1/2} \Big(h_\psi + h_c^2 + \|\tilde{\xi}_{e,m-1}\| + \|\tilde{\xi}_{e,m-2}\| \\
&\quad + \|\tilde{\xi}_{p,m-1}\| + \|\tilde{\xi}_{p,m-2}\| \Big) \Big(\|\xi_e^n\| + \|\zeta_e^n\| \Big) \\
&\le K h_c^{-1} \Big(h_\psi^2 + h_c^4 + \|\tilde{\xi}_{e,m-1}\|^2 + \|\tilde{\xi}_{e,m-2}\|^2 + \|\tilde{\xi}_{p,m-1}\|^2 + \|\tilde{\xi}_{p,m-2}\|^2 \Big) \|D_e^{-1/2} \zeta_e^{n-1}\|^2 \\
&\quad + h_c^{-1/2} \Big(h_\psi + h_c^2 + \|\tilde{\xi}_{e,m-1}\| + \|\tilde{\xi}_{e,m-2}\| \\
&\quad + \|\tilde{\xi}_{p,m-1}\| + \|\tilde{\xi}_{p,m-2}\| \Big) \Big(\|D_e^{-1/2} \zeta_e^{n-1}\|^2 + \|D_e^{-1/2} \zeta_e^n\|^2 \Big) + K \|\xi_e^n\|^2. \qquad (4.21)
\end{aligned}
$$

Furthermore, the induction hypothesis (4.13) and the condition $h_\psi = O(h_c^{3/2})$ give us

$$
|T_9| \le \varepsilon \Big(\|D_e^{-1/2} \zeta_e^{n-1}\|^2 + \|D_e^{-1/2} \zeta_e^n\|^2 \Big) + K \|\xi_e^n\|^2. \qquad (4.22)
$$

For T_{10}, we use Lemma 3.3 to obtain

$$
\begin{aligned}
|T_{10}| &\le (\Delta t_c)^{-1} \Big(|(\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}, \Phi_e^n)| + |(\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}, \xi_e^n - \Phi_e^n)| \Big) \\
&\le (\Delta t_c)^{-1} \Big(\|\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}\|_{-1} \|\Phi_e^n\|_1 + \|\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}\| \|\xi_e^n - \Phi_e^n\| \Big) \\
&\le (\Delta t_c)^{-1} \Big(\|\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}\|_{-1} + h_c \|\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}\| \Big) \Big(\|\xi_e^n\|_{-1} + \|\zeta_e^n\| \Big). \qquad (4.23)
\end{aligned}
$$

From [5, 9] we have

$$
\|\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}\|_{-1} \le K \|\tilde{\eta}_e^{n-1}\| \Delta t_c,
$$

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and we see that

$$\|\tilde{\eta}_e^{n-1} - \check{\tilde{\eta}}_e^{n-1}\| \le K\|\tilde{\eta}_e^{n-1}\|.$$

Now, substitute the above two estimates into (4.23) and then use (3.3c) and ε-Cauchy inequality to obtain

$$\begin{aligned}|T_{10}| &\le K\Big(\|\tilde{\eta}_e^{n-1}\| + \|\tilde{\eta}_e^{n-1}\|(\Delta t_c)^{-1}h_c\Big)\{\|\xi_e^n\|_{-1} + \|\zeta_e^n\|\}\\ &\le \varepsilon\|D_e^{-1/2}\zeta_e^n\|^2 + K\Big(h_c^4 + h_c^6(\Delta t_c)^{-2} + \|\xi_e^n\|^2\Big). \end{aligned} \tag{4.24}$$

For the last term T_{11}, by Lemma 3.3 and (3.5c), we have

$$\begin{aligned}|T_{11}| &\le K\left(\|\tilde{\xi}_e^{n-1}\| + \left(\sum_{\mathcal{B}\in\mathcal{T}_h}\|\nabla\tilde{\xi}_e^{n-1}\|_{\mathcal{B}}^2\right)^{1/2}(\Delta t_c)^{-1}h_c^2\right)\Big(\|\xi_e^n\|_{-1} + \|\zeta_e^n\|\Big)\\ &\le K\Big((\Delta t_c)^{-2}h_c^4\Big(\|D_e^{-1/2}\zeta_e^{n-1}\|^2 + \|D_e^{-1/2}\zeta_e^n\|^2\Big) + \|\tilde{\xi}_e^{n-1}\|^2 + \|\xi_e^n\|^2\Big). \end{aligned} \tag{4.25}$$

Assembling (4.9), (4.10)$\sim$(4.12), (4.14)$\sim$(4.17), (4.19), (4.20), (4.22), (4.24) and (4.25), we obtain

$$\begin{aligned}&\frac{1}{2\Delta t_c}\Big[(\tilde{\xi}_e^n,\tilde{\xi}_e^n) - (\tilde{\xi}_e^{n-1},\tilde{\xi}_e^{n-1})\Big] + \frac{1}{2\Delta t_c}(2\Delta t_c - K_3'h_c^2)(D_e^{-1/2}\zeta_e^n,\zeta_e^n)\\ &\le K\left(\left\|\frac{\partial^2 e}{\partial\check{\tau}_e^2}\right\|^2_{L^2(t^{n-1},t^n;L^2)} + \left\|\frac{\partial e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;L^2)}\right)\Delta t_c\\ &\quad + K\left(\left\|\frac{\partial^2 u}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_m;L^2)} + \left\|\frac{\partial^2 u}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_m;H(\mathrm{div}))}\right)(\Delta t_\psi)^3\\ &\quad + K\left(\left\|\frac{\partial e}{\partial\check{\tau}_e}\right\|^2_{L^2(t^{n-1},t^n;L^2)} + \left\|\frac{\partial p}{\partial\check{\tau}_p}\right\|^2_{L^2(t^{n-1},t^n;L^2)}\right)(\Delta t_c)^2\\ &\quad + K\Big(\|z_e\|^2_{L^2(t^{n-1},t^n;H^1)} + \|\nabla\cdot z_e\|^2_{L^2(t^{n-1},t^n;H^1)}\\ &\quad + \left\|\frac{\partial z_e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;H^1)} + \left\|\nabla\cdot\frac{\partial z_e}{\partial t}\right\|^2_{L^2(t^{n-1},t^n;H^1)}\Big)(\Delta t_c)^{-1}h_c^4\\ &\quad + K\Big(h_\psi^2 + h_c^4 + h_c^6(\Delta t_c)^{-2}\Big) + K\Big(\|\tilde{\xi}_{e,m-1}\|^2 + \|\tilde{\xi}_{e,m-2}\|^2\\ &\quad + \|\tilde{\xi}_{p,m-1}\|^2 + \|\tilde{\xi}_{p,m-2}\|^2 + \|\tilde{\xi}_e^{n-1}\|^2 + \|\tilde{\xi}_p^{n-1}\|^2 + \|\tilde{\xi}_e^n\|^2\Big)\\ &\quad + K(\Delta t_c)^{-2}h_c^4\Big(\|D_e^{-1/2}\zeta_e^{n-1}\|^2 + \|D_e^{-1/2}\zeta_e^n\|^2\Big)\\ &\quad + \varepsilon\|D_e^{-1/2}\zeta_e^{n-1}\|^2 + 4\varepsilon\|D_e^{-1/2}\zeta_e^n\|^2. \end{aligned} \tag{4.26}$$

By (4.1) and $\Delta t_c \ge K' h_c^{3/2}$, we deduce that

$$K_3'h_c^2 \le K_3'(K')^{-1}\Delta t_c h_c^{1/2}, \quad h_c^6(\Delta t_c)^{-2} \le (K')^{-4}(\Delta t_c)^2, \quad (\Delta t_c)^{-2}h_c^4 \le (K')^{-2}h_c.$$

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Multiply (4.26) by $2\Delta t_c$ and then sum it over $1 \le n \le l$. Choosing ε and h_c sufficiently small, and using Lemma 3.2, we obtain

$$\begin{aligned}&\|\tilde{\xi}_e^l\|^2 + \sum_{n=1}^{l} \|\zeta_e^n\|^2 \Delta t_c \\ &\le K\Big((\Delta t_c)^2 + (\Delta t_\psi)^4 + (\Delta t_\psi^1)^3 + h_c^3 + h_\psi^2\Big) + K\sum_{n=1}^{l}\Big(\|\tilde{\xi}_e^n\|^2 + \|\tilde{\xi}_p^n\|^2\Big)\Delta t_c. \end{aligned} \tag{4.27}$$

For the hole concentration equation, a same argument gives us

$$\begin{aligned}&\|\tilde{\xi}_p^l\|^2 + \sum_{n=1}^{l} \|\zeta_p^n\|^2 \Delta t_c \\ &\le K\Big((\Delta t_c)^2 + (\Delta t_\psi)^4 + (\Delta t_\psi^1)^3 + h_c^3 + h_\psi^2\Big) + K\sum_{n=1}^{l}\Big(\|\tilde{\xi}_e^n\|^2 + \|\tilde{\xi}_p^n\|^2\Big)\Delta t_c. \end{aligned} \tag{4.28}$$

Summing (4.27) and (4.28) and applying the discrete Gronwall lemma, we have

$$\begin{aligned}&\|\tilde{\xi}_e^l\|^2 + \|\tilde{\xi}_p^l\|^2 + \sum_{n=1}^{l} \|\zeta_e^n\|^2 \Delta t_c + \sum_{n=1}^{l} \|\zeta_p^n\|^2 \Delta t_c \\ &\le K\Big((\Delta t_c)^2 + (\Delta t_\psi)^4 + (\Delta t_\psi^1)^3 + h_c^3 + h_\psi^2\Big). \end{aligned} \tag{4.29}$$

To complete the proof, we turn to check the induction hypothesis (4.13). Since $\tilde{\xi}_e^0 = \tilde{\xi}_p^0 = 0$, we get $h_c^{-1}\|\tilde{\xi}_e^0\|^2 = h_c^{-1}\|\tilde{\xi}_p^0\|^2 = 0$. It follows from (4.29) and (4.1) that

$$h_c^{-1}\|\tilde{\xi}_s^l\|^2 \le K h_c^{-1}\Big((\Delta t_c)^2 + (\Delta t_\psi)^4 + (\Delta t_\psi^1)^3 + h_c^3 + h_\psi^2\Big) \to 0, \quad h_c \to 0, \quad s = e, p.$$

Thus, (4.29) holds for all concentration time levels.

Finally, (4.29) and (3.3) yield (4.2)$\sim$(4.4), the desired results. □

Combining (3.7), (3.8) and (4.2), we obtain at once the following bound for approximations of the electric field intensity and the electrostatic potential.

Corollary 4.1. *Supposing that the assumptions of Theorem* 4.1 *hold, we have*

$$\begin{aligned}&\max_{1\le m\le M}\Big(\|u_{hm} - u_m\|_{H(\mathrm{div})} + \|\psi_{hm} - \psi_m\|\Big) \\ &\le K\Big(h_c^{3/2} + h_\psi + \Delta t_c + (\Delta t_\psi)^2 + (\Delta t_\psi^1)^{3/2}\Big). \end{aligned}$$

5. Numerical experiments

5.1. Numerical example 1

First, we assume that u is known and focus on the characteristics-mixed finite element approximation combined with a post-processing step for approximating convection-

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Table 1: Numerical results of $\|e - e_h\|_h$ for example 1.

	$h = 1/4$	$h = 1/8$	$h = 1/16$
$\epsilon = 1$	8.37936e-003	2.04794e-003 2.03	4.46738e-004 2.20
$\epsilon = 10^{-3}$	1.46724e-002	3.77369e-003 1.96	9.62809e-004 1.97
$\epsilon = 10^{-8}$	1.46678e-002	3.75608e-003 1.97	9.41237e-004 2.00

Table 2: Numerical results of $\|z_e - z_{eh}\|_h$ for example 1.

	$h = 1/4$	$h = 1/8$	$h = 1/16$
$\epsilon = 1$	1.28241e-003	3.07871e-004 2.06	6.83190e-005 2.17
$\epsilon = 10^{-3}$	2.88104e-003	9.02797e-004 1.67	2.32485e-004 1.96
$\epsilon = 10^{-8}$	2.89707e-003	9.13636e-004 1.66	2.42117e-004 1.92

dominated diffusion problem. We consider

$$\begin{cases} \dfrac{\partial e}{\partial t} + u \cdot \nabla e - \dfrac{\epsilon}{3\pi^2}\Delta e = f, & x \in \Omega,\ 0 < t \le T, \\ e(x,0) = e_0, & x \in \Omega, \\ \dfrac{\partial e}{\partial \nu} = 0, & x \in \partial\Omega,\ 0 < t \le T, \end{cases} \tag{5.1}$$

where $\Omega = (0,1)\times(0,1)\times(0,1)$ and ν is the unit outward normal vector on boundary $\partial\Omega$. $u = (u_1, u_2, u_3)$ and

$$\begin{aligned} u_1 &= \exp(-\epsilon t)\sin(\pi x_1)\cos(\pi x_2)\cos(\pi x_3)/(3\pi), \\ u_2 &= \exp(-\epsilon t)\cos(\pi x_1)\sin(\pi x_2)\cos(\pi x_3)/(3\pi), \\ u_3 &= \exp(-\epsilon t)\cos(\pi x_1)\cos(\pi x_2)\sin(\pi x_3))/(3\pi). \end{aligned}$$

We choose f and e_0 such that the exact solution is $e = \exp(-\epsilon t)\cos(\pi x_1)\cos(\pi x_2)\cos(\pi x_3)$. We approximate (5.1) by using the characteristics-mixed finite element method, which has been employed to discretize the electron and hole concentration equations in our paper. We set $\Delta t = 0.001$ and $t = 1.0$. We numerically solve (5.1) for $\epsilon = 1, 10^{-3}, 10^{-8}$, respectively. The numerical results of the errors $\|e - e_h\|_h$ and $\|z_e - z_{eh}\|_h$ are presented in Tables 1-2, where $\|\cdot\|_h$ denotes the approximate L^2-norm defined by using numerical integration. We can see that the errors decrease by a satisfactory factor as the space step h decreases by a factor of two. This indicates that all errors converge at rates of no less than first-order. The comparison sectional drawings of e and e_h at $x_3 = 0.28125$ for

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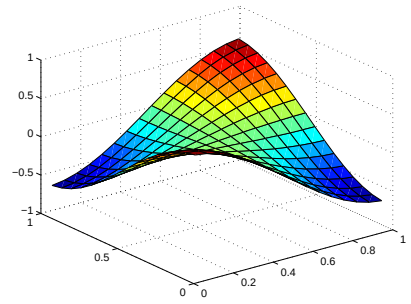


Figure 1: The sectional drawing of e, at $t = 1$, for $h = 1 = 16$.

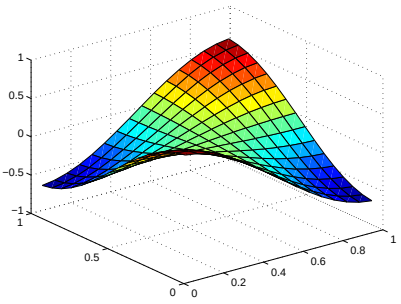


Figure 2: The sectional drawing of e_h, at $t = 1$, for $h = 1 = 16$.

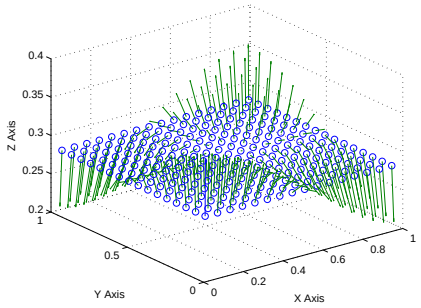


Figure 3: The quiver plot of z_e, at $t = 1$, for $h = 1/16$.

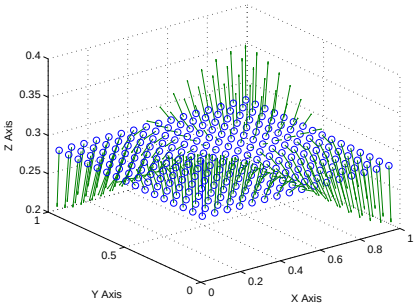


Figure 4: The quiver plot of z_{eh}, at $t = 1$, for $h = 1/16$.

$\epsilon = 10^{-3}$ are presented in Figures 1-2. Figures 3-4 show the comparison quiver plots of z_e and z_{eh} at the section $x_3 = 0.28125$ for $\epsilon = 10^{-3}$.

Remark 5.1. From Tables 1-2 and Figures 1-4, we can see that the method is stable and capable of approximating e and z_e simultaneously. It is also shown that our method is efficient for small ϵ.

5.2. Numerical example 2

Now, we solve a system consisting of an elliptic equation and a convection-diffusion equation. We consider

$$\begin{cases} -\Delta\psi = \nabla \cdot u = e + F, & x \in \partial\Omega,\ 0 \le t \le T, \\ \dfrac{\partial e}{\partial t} + u \cdot \nabla e - \epsilon \Delta e = f, & x \in \Omega,\ 0 < t \le T, \\ e(x,0) = e_0, & x \in \Omega, \\ \dfrac{\partial e}{\partial \nu} = 0, & x \in \partial\Omega,\ 0 < t \le T, \\ -\dfrac{\partial \psi}{\partial \nu} = u \cdot \nu = 0, & x \in \partial\Omega,\ 0 < t \le T, \end{cases} \tag{5.2}$$

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Table 3: Numerical results for example 2.

	$h = 1/4$	$h = 1/8$	$h = 1/16$
$\|\psi - \psi_h\|_h$	1.82852e-004	1.17235e-004 0.64	3.30572e-005 1.82
$\|u - u_h\|_h$	6.95898e-003	1.86974e-003 1.90	4.74263e-004 1.98
$\|e - e_h\|_h$	1.39414e-001	8.76624e-002 0.67	4.46468e-002 0.97
$\|z - z_h\|_h$	1.78590e-003	8.88468e-004 1.01	4.85070e-004 0.87

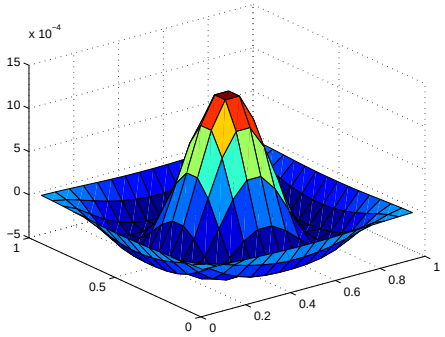


Figure 5: The sectional drawing of ψ, at $t = 1$, for $h = 1/16$.

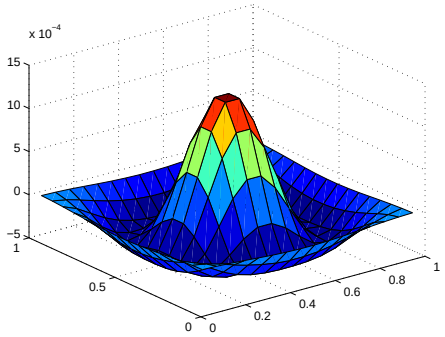


Figure 6: The sectional drawing of ψ_h, at $t = 1$, for $h = 1/16$.

where $\Omega = (0,1) \times (0,1) \times (0,1)$ and ν is the unit outward normal vector on boundary $\partial\Omega$. We choose F, f and e_0 such that exact solutions are

$$\psi = e^{12t}\big(x_1^4(1-x_1)^4x_2^4(1-x_2)^4x_3^4(1-x_3)^4 - x_1^2(1-x_1)^2x_2^2(1-x_2)^2x_3^2(1-x_3)^2/21^3\big),$$

$$e = -e^{12t}\sum_{i=1}^{3}\Big(12x_i^2(1-x_i)^4 - 32x_i^3(1-x_i)^3 + 12x_i^4(1-x_i)^2\Big) \cdot x_{i+1}^4(1-x_{i+1})^4x_{i+2}^4(1-x_{i+2})^4,$$

where $x_4 = x_1$ and $x_5 = x_2$. We apply mixed finite element method to approximate the first equation in (5.2), and the characteristics-mixed finite element method to approximate the second one. The numerical results for $\epsilon = 10^{-3}$ are showed in table 3, and the comparison plots are provided in Figures 5-12.

Remark 5.2. From Table 3 and Figures 5-12, we can conclude that the combined numerical method is effective to treat the system as (5.2).

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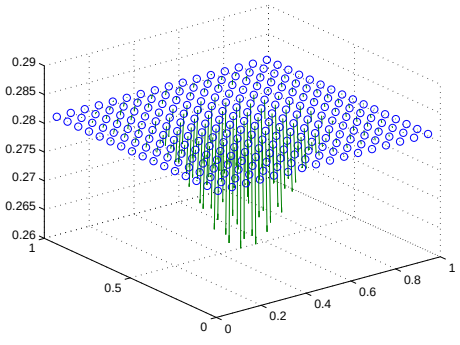


Figure 7: The quiver plot of u, at $t = 1$, for $h = 1/16$.

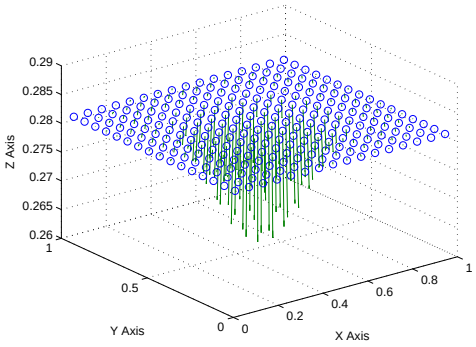


Figure 8: The quiver plot of u_h, at $t = 1$, for $h = 1/16$.

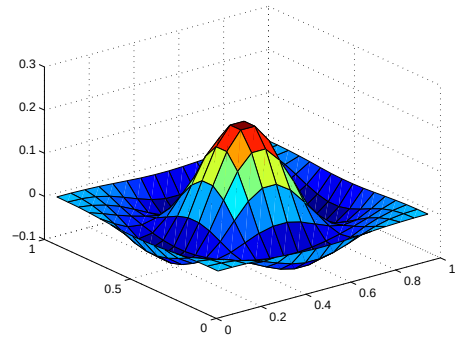


Figure 9: The sectional drawing of e, at $t = 1$, for $h = 1/16$.

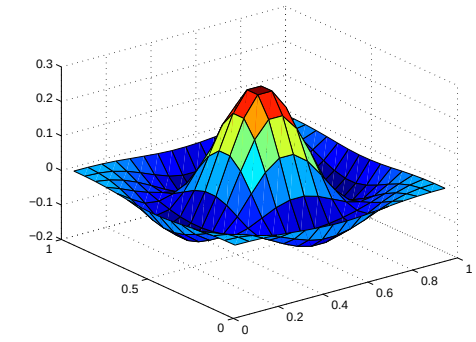


Figure 10: The sectional drawing of e_h, at $t = 1$, for $h = 1/16$.

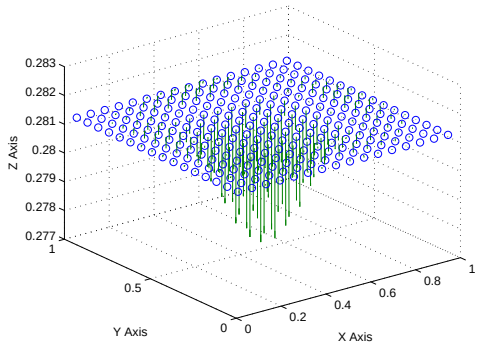


Figure 11: The quiver plot of z, at $t = 1$, for $h = 1/16$.

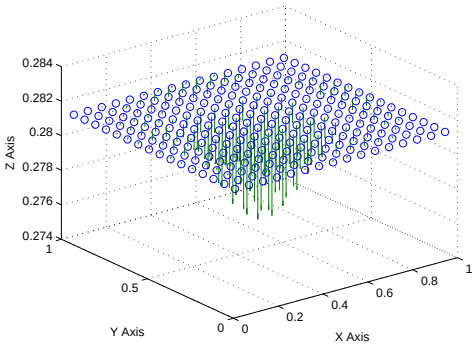


Figure 12: The quiver plot of z_h, at $t = 1$, for $h = 1/16$.

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