

TWO-GRID METHOD FOR SEMICONDUCTOR DEVICE PROBLEM BY MIXED FINITE ELEMENT METHOD AND CHARACTERISTICS FINITE ELEMENT METHOD

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ABSTRACT. The mathematical model of a semiconductor device is described by a coupled system of three quasilinear partial differential equations. The mixed finite element method is presented for the approximation of the electrostatic potential equation, and the characteristics finite element method is used for the concentration equations. First, we estimate the mixed finite element and the characteristics finite element method solution in the sense of the L^q norm. To linearize the full discrete scheme of the problem, we present an efficient two-grid method based on the idea of Newton iteration. The two-grid algorithm is to solve the nonlinear coupled equations on the coarse grid and then solve the linear equations on the fine grid. Moreover, we obtain the L^q error estimates for this algorithm. It is shown that a mesh size satisfies $H = O(h^{1/2})$ and the two-grid method still achieves asymptotically optimal approximations. Finally, the numerical experiment is given to illustrate the theoretical results.

1. Introduction. In this study, we consider the following mathematical model of a semiconductor device, which consists of three quasilinear partial differential equations [1, 15]:

$$-\Delta\psi = \alpha(p - e + N(x)), \quad (x, t) \in \Omega \times J, J = (0, T], \quad (1)$$

$$\frac{\partial e}{\partial t} = \nabla \cdot [D_e(x)\nabla e - \mu_e(x)e\nabla\psi] - R(e, p), (x, t) \in \Omega \times J, \quad (2)$$

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$$\frac{\partial p}{\partial t} = \nabla \cdot [D_p(x)\nabla p + \mu_p(x)p\nabla\psi] - R(e, p), (x, t) \in \Omega \times J, \quad (3)$$

where (1) is an elliptic-type partial differential equation for the electric potential, and (2) and (3) are parabolic-type partial differential equations for the electron and hole concentrations. The unknown functions are the electrostatic potential ψ , the electron concentration e , and the hole concentration p . Ω is a polygonal domain in $\mathbb{R}^d (d = 2, 3)$. The value of α is q/ϵ , q is the electron charge, and ϵ is the dielectric permittivity. These are all positive constants. $N(x) = N_D(x) - N_A(x)$ is a given function of $N_D(x)$ and $N_A(x)$ that represents the donor and acceptor impurity concentrations. The diffusion coefficients $D_s(x) (s = e, p)$ and the mobilities $\mu_s(x) (s = e, p)$ obey the Einstein relation $D_s(x) = U_T \mu_s(x)$, where U_T is the thermal voltage. $R(e, p)$ is a recombination term.

It is assumed that the boundary and initial conditions are as follows:

$$\psi(x, t) = e(x, t) = p(x, t) = 0, \quad (x, t) \in \partial\Omega \times J, \quad (4)$$

$$e(x, 0) = e_0(x), \quad p(x, 0) = p_0(x), \quad x \in \Omega. \quad (5)$$

In addition, we need the compatibility condition

$$\int_{\Omega} (p_0 - e_0 + N) dx = 0. \quad (6)$$

The study of the transient behaviors of semiconductor devices plays an important role in modern computational mathematics. Since Gummel [14] first presented sequence iterative computation methods for this kind of problem in 1964, a variety of numerical approaches have been introduced to obtain better approximations for (1)–(3). The main techniques include the difference method [13], finite element method [27], mixed finite element method [25], characteristics finite element method [26], characteristics finite difference method [24], upwind finite volume method [21], and characteristics mixed finite element method [22].

The semiconductor device problem becomes a large system of non-linear equations when using the finite element method to solve (1)–(5). Thus, we will consider a highly efficient and accurate algorithm for this large system. It is well known that the two-grid algorithm is a simple but effective algorithm. This method was first proposed by Xu for non-linear elliptic equations [18, 19] and has been widely used in many kinds of problems. Dawson [10] applied a two-grid finite difference scheme for non-linear parabolic equations. Chen [6, 5] presented an efficient two-grid scheme for semi-linear reaction–diffusion equations and miscible displacement problems. Dai [9] used a two-grid method based on Newton iteration for the Navier–Stokes equations. Chen and Yang [4] introduced this method for finite volume element approximations of nonlinear parabolic equations. Yu [23] presented a two-grid algorithm for mixed Stokes–Darcy problem. Wang investigated this method for semi-linear elliptic interface problem [16]. Xu and Hou recently used this method for semilinear parabolic integro–differential equations [20]. Thus, it would be natural to use the two-grid method for the equations of a semiconductor device.

The electric field intensity $\mathbf{u} = -\nabla\psi$ is very important in production, and the numerical behavior of (2) and (3) strongly depends on the accuracy of the approximation of \mathbf{u} . To improve the accuracy of e and p , we apply the mixed finite element method, which gives direct approximations of ψ and \mathbf{u} simultaneously for the electric potential equation (1). The direct approximation of the electric field intensity, rather than one that requires differentiation of ψ , can provide improved accuracy for the same computational effort.

We use the characteristics finite element method for the electron and hole concentration equations, (2) and (3), respectively. In reality, the values of D_s ($s = e, p$) are quite small in the concentration equations, and thus, (2) and (3) are strongly convection dominated. The standard finite element method produces unacceptable numerical diffusion or nonphysical oscillations in the concentration approximation. The characteristics finite element method was introduced and analyzed by Douglas and Russell [12] in 1982. Using this method to treat the hyperbolic parts of the concentration equation, the procedure is simple, the time-truncation errors are smaller, and lastly and most importantly, nonphysical oscillations are avoided.

We determine the L^q error estimates for the mixed finite element solutions and the characteristics finite element solutions. We then present an efficient two-grid method based on the idea of Newton iteration. To the best of our knowledge, few results about the application of the two-grid algorithm to semiconductor device problems have been reported. The main idea of this algorithm is to solve the nonlinear coupled equations on a coarse grid, and then to solve the linear equations on a fine grid rather than solving the coupled nonlinear equations on the fine grid. Finally, we obtain the L^q error estimates for this algorithm and give the numerical experiment to illustrate the theoretical results. The two-grid algorithm achieves asymptotically optimal approximations but requires less time.

An outline of this paper is as follows. In Section 2, we present the weak formulation and full discrete scheme of this model. In Section 3, we present the L^q error estimates of the finite element solutions. In Section 4, we introduce a two-grid algorithm and analyze its convergence. Finally, the numerical experiment is presented in Section 5.

2. Weak formulation and full discrete scheme.

2.1. Notation and assumptions. In this paper, we denote $L^q(\Omega) = \{f : \|f\|_{L^q(\Omega)} < \infty\}$, where

$$\|f\|_{L^q(\Omega)} = \begin{cases} (\int_{\Omega} |f(x)|^q dx)^{1/q}, & 1 \leq q < \infty, \\ \text{ess sup}_{x \in \Omega} |f(x)|, & q = \infty. \end{cases}$$

$(L^2(\Omega))^2$ is the space of vectors that contains each component in $L^2(\Omega)$. We define the Sobolev spaces as $W^{m,q}(\Omega) = \{f \in L^1_{loc}(\Omega) : \|f\|_{W^{m,q}(\Omega)} < \infty\}$, whose norms are

$$\|f\|_{W^{m,q}(\Omega)} = \|f\|_{m,q} = \begin{cases} (\sum_{|\alpha| \leq m} \|\partial^\alpha f\|_{L^q(\Omega)}^q)^{1/q}, & 1 \leq q < \infty, \\ \max_{|\alpha| \leq m} \|\partial^\alpha f\|_{L^\infty(\Omega)}, & q = \infty. \end{cases}$$

To simplify the notation, we write $H^m(\Omega) = W^{m,2}(\Omega)$, $\|\cdot\|_m = \|\cdot\|_{m,2}$ and $\|\cdot\| = \|\cdot\|_{0,2}$. Let X be any of the spaces just defined. If $f(x, t)$ represents functions on $\Omega \times J$, we set

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

$$\|f\|_{H^m(J; X)} = \left[\sum_{\alpha=0}^m \int_J \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X^2 dt \right]^{\frac{1}{2}}, \quad m \geq 0,$$

$$\begin{aligned}
W^{m,\infty}(J; X) &= \left\{ f : \operatorname{ess\,sup}_{t \in J} \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X < \infty, \quad \alpha \leq m \right\}, \\
\|f\|_{W^{m,\infty}(J; X)} &= \max_{0 \leq \alpha \leq m} \operatorname{ess\,sup}_{t \in J} \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X, \quad m \geq 0, \\
L^2(J; X) &= H^0(J; X), \quad L^\infty(J; X) = W^{0,\infty}(J; X).
\end{aligned}$$

For convenience, we drop Ω from the notations. Thus, we write $L^\infty(J; H^{k+3})$ for $L^\infty(J; H^{k+3}(\Omega))$.

We let (\cdot, \cdot) be the $L^2(\Omega)$ inner product. Furthermore, $H_0^1(\Omega) = \{f \in H^1(\Omega) : f|_{\partial\Omega} = 0\}$, and $H(\operatorname{div}; \Omega)$ is the set of vector functions in $(L^2(\Omega))^2$ that have $\nabla \cdot \mathbf{v} \in L^2(\Omega)$. We also define

$$\begin{aligned}
W &= \{w \in L^2(\Omega), (w, 1) = 0\}, \\
\mathbf{V} &= H(\operatorname{div}; \Omega), \\
\|\mathbf{v}\|_{\mathbf{V}} &= \|\mathbf{v}\|_{H(\operatorname{div}; \Omega)} = (\|\mathbf{v}\|^2 + \|\nabla \cdot \mathbf{v}\|^2)^{1/2}.
\end{aligned}$$

We provide some rational assumptions about the coefficients and the solutions of (1)–(3). These assumptions are reasonable in physics [15, 14].

(1) For integers $l, k \geq 0$, the solution functions have the following regularity (A) $\psi \in L^\infty(J; H^{k+3})$; $\mathbf{u} \in (L^\infty(J; H^{k+2}))^2$; $e, p \in W^{1,\infty}(J; H^{l+1}) \cap H^2(J; W^{1,\infty})$.

(2) The problem is positive definite, such that

$$0 < D_* \leq D_s(x) \leq D^*, \quad 0 < \mu_* \leq \mu_s(x) \leq \mu^*, \quad s = e, p,$$

where D_* , D^* , μ_* , and μ^* are positive constants.

(3) $|\nabla \mu_s(x)| \leq C$, $s = e, p$.

(4) $R(e, p)$ is Lipschitz continuous in an ε -neighborhood of the solutions.

2.2. Characteristics method for the concentration equations. For the electron and hole concentration equations, (2) and (3), respectively, convection is dominant over diffusion, so we use the characteristics finite element method to solve them.

We rewrite (2) and (3) in the form

$$\frac{\partial e}{\partial t} = \nabla \cdot (D_e \nabla e) + e \mathbf{u} \cdot \nabla \mu_e + \mu_e \nabla e \cdot \mathbf{u} + \alpha \mu_e e(p - e + N) - R(e, p), \quad (7)$$

$$\frac{\partial p}{\partial t} = \nabla \cdot (D_p \nabla p) - p \mathbf{u} \cdot \nabla \mu_p - \mu_p \nabla p \cdot \mathbf{u} - \alpha \mu_p p(p - e + N) - R(e, p), \quad (8)$$

where $\mathbf{u} = -\nabla \psi$.

We let $\mathbf{u} = (u_1, u_2)^T$, τ_e be the unit vector in the direction $(-\mu_e u_1, -\mu_e u_2, 1)$, τ_p be the unit vector in the direction $(\mu_p u_1, \mu_p u_2, 1)$, and $\phi_s = \sqrt{1 + \mu_s^2(u_1^2 + u_2^2)}$ ($s = e, p$). The characteristic derivatives in the t direction are given by

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

Associated with the equations above, (7) and (8) can be rewritten as follows:

$$\phi_e \frac{\partial e}{\partial \tau_e} - \nabla \cdot (D_e \nabla e) - e \mathbf{u} \cdot \nabla \mu_e - \alpha \mu_e e(p - e + N) = -R(e, p), \quad (9)$$

$$\phi_p \frac{\partial p}{\partial \tau_p} - \nabla \cdot (D_p \nabla p) + p \mathbf{u} \cdot \nabla \mu_p + \alpha \mu_p p(p - e + N) = -R(e, p). \quad (10)$$

We partition J into $\Delta t = T/N$ and $t^n = n\Delta t$. Furthermore, we denote $f^n(x)$ as $f(x, t^n)$ and $(\partial e^n / \partial \tau_e)(x)$ as $(\partial e / \partial \tau_e)(x, t^n)$. The backward difference quotient in the τ_e -direction is as follows:

$$\frac{\partial e^n}{\partial \tau_e}(x) \approx \frac{e^n(x) - e^{n-1}(x + \mu_e \mathbf{u}^n(x) \Delta t)}{\Delta t \sqrt{1 + \mu_e^2 |\mathbf{u}^n(x)|^2}}.$$

Defining $\hat{x}_e^{n-1} = x + \mu_e \mathbf{u}^n(x) \Delta t$ and $\hat{e}^{n-1}(x) = e^{n-1}(\hat{x}_e^{n-1})$, then

$$\phi_e^n \frac{\partial e^n}{\partial \tau_e} \approx \frac{e^n - \hat{e}^{n-1}}{\Delta t}. \quad (11)$$

Similarly,

$$\frac{\partial p^n}{\partial \tau_p}(x) \approx \frac{p^n(x) - p^{n-1}(x - \mu_p \mathbf{u}^n(x) \Delta t)}{\Delta t \sqrt{1 + \mu_p^2 |\mathbf{u}^n(x)|^2}}.$$

Defining $\hat{x}_p^{n-1} = x - \mu_p \mathbf{u}^n(x) \Delta t$ and $\hat{p}^{n-1}(x) = p^{n-1}(\hat{x}_p^{n-1})$, then

$$\phi_p^n \frac{\partial p^n}{\partial \tau_p} \approx \frac{p^n - \hat{p}^{n-1}}{\Delta t}. \quad (12)$$

2.3. Weak form and full discrete procedure. The weak forms of (1), (9) and (10) are equivalent to the following problem: for $t \in J$, find a map $\{\psi, \mathbf{u}, e, p\} : J \rightarrow W \times \mathbf{V} \times H_0^1(\Omega) \times H_0^1(\Omega)$ such that $e(x, 0) = e_0(x)$, $p(x, 0) = p_0(x)$:

$$(\mathbf{u}, \mathbf{v}) - (\nabla \cdot \mathbf{v}, \psi) = 0, \quad \forall \mathbf{v} \in \mathbf{V}, \quad (13)$$

$$(\nabla \cdot \mathbf{u}, w) = \alpha(p - e + N, w), \quad \forall w \in W, \quad (14)$$

$$\begin{aligned} & (\phi_e \frac{\partial e}{\partial \tau_e}, z) + (D_e \nabla e, \nabla z) - (e \mathbf{u} \cdot \nabla \mu_e, z) - \alpha(\mu_e e(p - e + N), z) \\ &= -(R(e, p), z), \quad \forall z \in H_0^1(\Omega), \end{aligned} \quad (15)$$

$$\begin{aligned} & (\phi_p \frac{\partial p}{\partial \tau_p}, z) + (D_p \nabla p, \nabla z) + (p \mathbf{u} \cdot \nabla \mu_p, z) + \alpha(\mu_p p(p - e + N), z) \\ &= -(R(e, p), z), \quad \forall z \in H_0^1(\Omega). \end{aligned} \quad (16)$$

We let \mathcal{T}_{h_ψ} and \mathcal{T}_{h_c} be a quasi-uniform mesh of Ω comprising triangles or rectangles such that the elements have diameters bounded by h_ψ and h_c . We denote $W_h \times \mathbf{V}_h \subset W \times \mathbf{V}$ as the Raviart–Thomas mixed finite element spaces with order k . The approximation properties are given as follows:

$$\begin{aligned} \inf_{\mathbf{v}_h \in \mathbf{V}_h} \|\mathbf{v} - \mathbf{v}_h\|_{L^2(\Omega)^2} &\leq C \|\mathbf{v}\|_{k+1} h_\psi^{k+1}, \\ \inf_{\mathbf{v}_h \in \mathbf{V}_h} \|\mathbf{v} - \mathbf{v}_h\|_{\mathbf{V}} &\leq C \{\|\mathbf{v}\|_{k+1} + \|\nabla \cdot \mathbf{v}\|_{k+1}\} h_\psi^{k+1}, \\ \inf_{w_h \in W_h} \|w - w_h\|_W &\leq C \|w\|_{k+1} h_\psi^{k+1}. \end{aligned}$$

We denote $M_h \subset H_0^1(\Omega)$ as a piecewise polynomial space of degree l , and

$$\inf_{z_h \in M_h} \|z - z_h\|_{1,q} \leq C \|z\|_{l+1,q} h_c^l, \quad \forall z \in H_0^{l+1}(\Omega).$$

Using (11) and (12), the full discrete scheme of the weak form, (13)–(16), consists of $\{\psi_h^n, \mathbf{u}_h^n, e_h^n, p_h^n\} \in W_h \times \mathbf{V}_h \times M_h \times M_h$, given by

$$(\mathbf{u}_h^n, \mathbf{v}) - (\nabla \cdot \mathbf{v}, \psi_h^n) = 0, \quad \forall \mathbf{v} \in \mathbf{V}_h, \quad (17)$$

$$(\nabla \cdot \mathbf{u}_h^n, w) = \alpha(p_h^n - e_h^n + N, w), \quad \forall w \in W_h, \quad (18)$$

$$\begin{aligned} & (\partial_{\tau_e} e_h^n, z) + (D_e \nabla e_h^n, \nabla z) - (e_h^n \mathbf{u}_h^n \cdot \nabla \mu_e, z) - \alpha(\mu_e e_h^n (p_h^n - e_h^n + N), z) \\ &= -(R(e_h^n, p_h^n), z), \quad \forall z \in M_h, \end{aligned} \quad (19)$$

$$\begin{aligned} & (\partial_{\tau_p} p_h^n, z) + (D_p \nabla p_h^n, \nabla z) + (p_h^n \mathbf{u}_h^n \cdot \nabla \mu_p, z) + \alpha(\mu_p p_h^n (p_h^n - e_h^n + N), z) \\ &= -(R(e_h^n, p_h^n), z), \quad \forall z \in M_h, \end{aligned} \quad (20)$$

where $\partial_{\tau_e} e_h^n = \frac{e_h^n - e_h^{n-1}}{\Delta t}$ and $\partial_{\tau_p} p_h^n = \frac{p_h^n - p_h^{n-1}}{\Delta t}$. In addition, the initial approximations e_h^0 and p_h^0 must be determined by the elliptic projections of e_0 and p_0 .

3. L^q error estimate of finite element solution. In this section, we present the L^q error estimate of the mixed finite element method for the electrostatic potential and electric field intensity and the characteristics finite element method for the concentrations.

3.1. Convergence analysis of mixed finite element solution. First, it is useful to introduce an elliptic mixed method projection $(R_h \psi, R_h \mathbf{u}) : J \rightarrow W_h \times \mathbf{V}_h$, which satisfies

$$(R_h \mathbf{u}, \mathbf{v}) - (\nabla \cdot \mathbf{v}, R_h \psi) = 0, \quad \forall \mathbf{v} \in \mathbf{V}_h, \quad (21)$$

$$(\nabla \cdot R_h \mathbf{u}, w) = \alpha(p - e + N, w), \quad \forall w \in W_h. \quad (22)$$

Following Brezzi [3], we have

$$\|\mathbf{u} - R_h \mathbf{u}\|_{\mathbf{V}} + \|\psi - R_h \psi\|_W \leq C \|\psi\|_{L^\infty(J; H^{k+3})} h_\psi^{k+1}. \quad (23)$$

The estimations of $\psi_h^n - R_h \psi^n$ and $\mathbf{u}_h^n - R_h \mathbf{u}^n$ are derived as follows. By subtracting (21) and (22) from (17) and (18), respectively, at time $t = t^n$, we determine that

$$(\mathbf{u}_h^n - R_h \mathbf{u}^n, \mathbf{v}) - (\nabla \cdot \mathbf{v}, \psi_h^n - R_h \psi^n) = 0, \quad \forall \mathbf{v} \in \mathbf{V}_h, \quad (24)$$

$$(\nabla \cdot (\mathbf{u}_h^n - R_h \mathbf{u}^n), w) = \alpha(p_h^n - p^n - e_h^n + e^n, w), \quad \forall w \in W_h. \quad (25)$$

Following Brezzi [3], we have

$$\|\mathbf{u}_h^n - R_h \mathbf{u}^n\|_{\mathbf{V}} + \|\psi_h^n - R_h \psi^n\|_W \leq C(\|e^n - e_h^n\| + \|p^n - p_h^n\|). \quad (26)$$

3.2. L^q error estimate of characteristics finite element method. We introduce an elliptic method projection $(R_h e, R_h p) : J \rightarrow M_h \times M_h$ such that

$$(D_e \nabla (R_h e - e), \nabla z) + \lambda_e (R_h e - e, z) = 0, \quad \forall z \in M_h, \quad (27)$$

$$(D_p \nabla (R_h p - p), \nabla z) + \lambda_p (R_h p - p, z) = 0, \quad \forall z \in M_h, \quad (28)$$

where the positive constants λ_s ($s = e, p$) will be chosen to ensure the coercivity of the forms. Based on the theory of the Galerkin method for elliptic problems [8, 17], we have

$$\|s - R_h s\|_{0,2} + h_c \|s - R_h s\|_{1,2} \leq C \|s\|_{l+1,2} h_c^{l+1}, \quad s = e, p. \quad (29)$$

To obtain the convergence estimations of $\|s^n - s_h^n\|_{0,q}(s = e, p)$, we divide them as follows:

$$\|s^n - s_h^n\|_{0,q} \leq \|s^n - R_h s^n\|_{0,q} + \|R_h s^n - s_h^n\|_{0,q}, \quad s = e, p. \quad (30)$$

For the concentration, we only discuss the electron concentration equation, as the results were similar for the hole concentration equation. First, we obtain the convergence results of $\|s^n - R_h s^n\|_{0,q}(s = e, p)$ with help of an elliptic problem.

Lemma 3.1. *If (e^n, p^n) is the solution of (15)–(16) at $t = t^n$, and $(R_h e^n, R_h p^n)$ is the elliptic projection solution of (27)–(28) at $t = t^n$, then for $1 \leq n \leq N$, $2 \leq q < \infty$ and $l \geq 1$, we have the following:*

$$\|e^n - R_h e^n\|_{0,q} \leq C \|e^n\|_{l+1,q} h_c^{l+1}, \quad (31)$$

$$\|p^n - R_h p^n\|_{0,q} \leq C \|p^n\|_{l+1,q} h_c^{l+1}. \quad (32)$$

Proof. We let L denote an elliptic operator such that

$$Le^n = -\nabla \cdot (D_e \nabla e^n) + \lambda e^n,$$

and it has a bilinear form

$$a(e^n, z) = (D_e \nabla e^n, \nabla z) + (\lambda e^n, z),$$

where λ will be chosen to ensure the coercivity of $a(e^n, z)$. From (27), it is clear that $R_h e^n$ is the finite element solution of this elliptic problem. We consider the auxiliary problem

$$\begin{aligned} L\omega &= \text{sgn}(e^n - R_h e^n) |e^n - R_h e^n|^{q-1}, \quad \text{in } \Omega, \\ \omega &= 0, \quad \text{on } \partial\Omega. \end{aligned}$$

This problem is uniquely solvable for $\omega \in L^p(\Omega)$, and

$$\|\omega\|_{2,p} \leq C \|L\omega\|_{0,p} = C \|e^n - R_h e^n\|_{0,q}^{q-1}, \quad (33)$$

where $\frac{1}{p} + \frac{1}{q} = 1$. We use a duality argument. Based on (27), Hölder's inequality, and (33), we denote I_h as an interpolation operator and obtain

$$\begin{aligned} \|e^n - R_h e^n\|_{0,q}^q &= a(e^n - R_h e^n, \omega) = a(e^n - R_h e^n, \omega - I_h \omega) \\ &\leq C \|e^n - R_h e^n\|_{1,q} \|\omega - I_h \omega\|_{1,p} \leq C h_c \|e^n - R_h e^n\|_{1,q} \|\omega\|_{2,p} \\ &\leq C h_c \|e^n - R_h e^n\|_{1,q} \|e^n - R_h e^n\|_{0,q}^{q-1}. \end{aligned} \quad (34)$$

From [2, Theorem 8.5.3] and the approximation property, we have

$$\|e^n - R_h e^n\|_{1,q} \leq C \inf_{e_h \in M_h} \|e^n - e_h\|_{1,q} \leq C h_c^l \|e^n\|_{l+1,q}. \quad (35)$$

Using (34) and (35), we have

$$\|e^n - R_h e^n\|_{0,q} \leq C h_c \|e^n - R_h e^n\|_{1,q} \leq C h_c^{l+1} \|e^n\|_{l+1,q}.$$

Lastly, we obtain similar results for the hole concentration equation. \square

Next, we obtain the convergence property for $\|R_h s^n - s_h^n\|_{0,q}(s = e, p)$.

Lemma 3.2. *Let $(R_h e^n, R_h p^n)$ be the elliptic projection solution of (27)–(28) at $t = t^n$, and (e_h^n, p_h^n) be the finite element solution of (19)–(20). If the regularity assumptions (A) hold, and the initial functions $e_h^0 = R_h e^0$ and $p_h^0 = R_h p^0$, then for $1 \leq n \leq N$, $2 \leq q < \infty$ and $l, k \geq 1$, we have*

$$\|e_h^n - R_h e^n\|_{0,q} \leq C (h_c^{l+1} + h_\psi^{k+1} + \Delta t), \quad (36)$$

$$\|p_h^n - R_h p^n\|_{0,q} \leq C (h_c^{l+1} + h_\psi^{k+1} + \Delta t). \quad (37)$$

Proof. The proof process is similar to the analysis presented by [25] and [26], but with some changes. First, we subtract (15) and (27) from (19) at $t = t^n$ to have

$$\begin{aligned} & (\partial_{\tau_e} e_h^n, z) - \left(\phi_e^n \frac{\partial e^n}{\partial \tau_e}, z \right) + (D_e \nabla(e_h^n - R_h e^n), \nabla z) \\ &= ((e_h^n \mathbf{u}_h^n - e^n \mathbf{u}^n) \cdot \nabla \mu_e, z) + \alpha(\mu_e[e_h^n(p_h^n - e_h^n + N) - e^n(p^n - e^n + N)], z) \\ & \quad + (R(e^n, p^n) - R(e_h^n, p_h^n), z) + \lambda_e(R_h e^n - e^n, z), \quad \forall z \in M_h. \end{aligned} \quad (38)$$

We let $\xi_e^n = e^n - R_h e^n$, $\zeta_e^n = e_h^n - R_h e^n$, $\xi_p^n = p^n - R_h p^n$, $\zeta_p^n = p_h^n - R_h p^n$, and select $z = \zeta_e^n - \zeta_e^{n-1} = \partial_t \zeta_e^n \Delta t$. Summing over $1 \leq n \leq m$, from (38), we have the following:

$$\sum_{n=1}^m (\partial_t \zeta_e^n, \partial_t \zeta_e^n) \Delta t + \frac{1}{2} (D_e \nabla \zeta_e^m, \nabla \zeta_e^m) - \frac{1}{2} (D_e \nabla \zeta_e^0, \nabla \zeta_e^0) \leq \sum_{i=1}^8 F_i, \quad (39)$$

where

$$\begin{aligned} F_1 &= \sum_{n=1}^m \left(R(e^n, p^n) - R(e_h^n, p_h^n), \partial_t \zeta_e^n \right) \Delta t, & F_2 &= \sum_{n=1}^m \left(\frac{\xi_e^n - \xi_e^{n-1}}{\Delta t}, \partial_t \zeta_e^n \right) \Delta t, \\ F_3 &= \sum_{n=1}^m \left(\frac{\zeta_e^{n-1} - \hat{\zeta}_e^{n-1}}{\Delta t}, \partial_t \zeta_e^n \right) \Delta t, & F_4 &= \sum_{n=1}^m \left(\frac{\hat{\zeta}_e^{n-1} - \zeta_e^{n-1}}{\Delta t}, \partial_t \zeta_e^n \right) \Delta t, \\ F_5 &= \sum_{n=1}^m \left(\phi_e^n \frac{\partial e^n}{\partial \tau_e} - \frac{e^n - \hat{e}^{n-1}}{\Delta t}, \partial_t \zeta_e^n \right) \Delta t, & F_6 &= - \sum_{n=1}^m \lambda_e(\xi_e^n, \partial_t \zeta_e^n) \Delta t, \\ F_7 &= \sum_{n=1}^m \left((e_h^n \mathbf{u}_h^n - e^n \mathbf{u}^n) \cdot \nabla \mu_e, \partial_t \zeta_e^n \right) \Delta t, \\ F_8 &= \sum_{n=1}^m \alpha \left(\mu_e[e_h^n(p_h^n - e_h^n + N) - e^n(p^n - e^n + N)], \partial_t \zeta_e^n \right) \Delta t. \end{aligned}$$

Now we estimate each term on the right hand of (39). First, using a second-order Taylor expansion at point (e_h^n, p_h^n) for $R(e^n, p^n)$, Young's inequality, and (29), we have

$$\begin{aligned} |F_1| &\leq \sum_{n=1}^m (\|R_e\|_{0,\infty} \|e^n - e_h^n\| + \|R_p\|_{0,\infty} \|p^n - p_h^n\|) \|\partial_t \zeta_e^n\| \Delta t \\ &\leq C \sum_{n=1}^m (\|\xi_e^n\| + \|\zeta_e^n\|) \|\partial_t \zeta_e^n\| \Delta t + C \sum_{n=1}^m (\|\xi_p^n\| + \|\zeta_p^n\|) \|\partial_t \zeta_e^n\| \Delta t \\ &\leq C(\varepsilon) \left(\sum_{n=1}^m (\|\zeta_e^n\|^2 + \|\zeta_p^n\|^2) \Delta t + h_c^{2l+2} \right) + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t, \end{aligned} \quad (40)$$

where R_e and R_p are the partial derivatives for each variable.

For F_2 , we have

$$\begin{aligned} |F_2| &\leq \sum_{n=1}^m \frac{C}{\Delta t} \int_{t^{n-1}}^{t^n} \left\| \frac{\partial \xi_e}{\partial t} \right\| dt \cdot \|\partial_t \zeta_e^n\| \Delta t \\ &\leq C(\varepsilon) \sum_{n=1}^m \left\| \frac{\partial \xi_e}{\partial t} \right\|_{L^2(t^{n-1}, t^n; L^2)}^2 + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t \end{aligned}$$

$$\leq C(\varepsilon)h_c^{2l+2}\|e\|_{H^1(t^{n-1}, t^n; H^{l+1})}^2 + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \quad (41)$$

For the estimation of F_3 , using (29), we get

$$\begin{aligned} |F_3| &\leq C(\varepsilon) \sum_{n=1}^m \|\nabla \zeta_e^{n-1}\|^2 \Delta t + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t \\ &\leq C(\varepsilon)h_c^{2l} + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \end{aligned} \quad (42)$$

As to F_4 , we obtain similar estimate:

$$|F_4| \leq C(\varepsilon) \sum_{n=1}^m \|\nabla \zeta_e^{n-1}\|^2 \Delta t + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \quad (43)$$

For F_5 , we obtain

$$\begin{aligned} |F_5| &\leq C(\varepsilon) \sum_{n=1}^m \left\| \phi_e^n \frac{\partial e^n}{\partial \tau_e} - \frac{e^n - \hat{e}^{n-1}}{\Delta t} \right\|^2 \Delta t + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t \\ &\leq C(\varepsilon)(\Delta t)^2 \left\| \frac{\partial^2 e}{\partial \tau_e^2} \right\|_{L^2(J; L^2(\Omega))}^2 + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t, \end{aligned} \quad (44)$$

where the calculations of (41), (42), and (44) are presented in detail elsewhere [25, 26].

For F_6 , from (29) we have

$$|F_6| \leq C(\varepsilon) \sum_{n=1}^m \|e^n - R_h e^n\| \|\partial_t \zeta_e^n\| \Delta t \leq C(\varepsilon)h_c^{2l+2} + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \quad (45)$$

Next, we obtain an error estimate for F_7 . Using (26), (29), and (23), we have

$$\begin{aligned} \|e_h^n \mathbf{u}_h^n - e^n \mathbf{u}^n\| &\leq \|(e_h^n - R_h e^n) \mathbf{u}_h^n\| + \|R_h e^n (\mathbf{u}_h^n - R_h \mathbf{u}^n)\| \\ &\quad + \|R_h \mathbf{u}^n (R_h e^n - e^n)\| + \|e^n (R_h \mathbf{u}^n - \mathbf{u}^n)\| \\ &\leq \|\mathbf{u}_h^n\|_{0,\infty} \|e_h^n - R_h e^n\| + \|R_h e^n\|_{0,\infty} \|\mathbf{u}_h^n - R_h \mathbf{u}^n\| \\ &\quad + \|R_h \mathbf{u}^n\|_{0,\infty} \|R_h e^n - e^n\| + \|e^n\|_{0,\infty} \|R_h \mathbf{u}^n - \mathbf{u}^n\| \\ &\leq C(\|\zeta_e^n\| + \|\zeta_p^n\| + h_c^{l+1} + h_\psi^{k+1}). \end{aligned}$$

Hence, we conclude that

$$\begin{aligned} |F_7| &\leq C \sum_{n=1}^m \|e_h^n \mathbf{u}_h^n - e^n \mathbf{u}^n\| \|\partial_t \zeta_e^n\| \Delta t \\ &\leq C(\varepsilon) \left(\sum_{n=1}^m (\|\zeta_e^n\|^2 + \|\zeta_p^n\|^2) \Delta t + h_c^{2l+2} + h_\psi^{2k+2} \right) + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \end{aligned} \quad (46)$$

Finally, for F_8 , we have

$$\begin{aligned} \|e_h^n (p_h^n - e_h^n + N) - e^n (p^n - e^n + N)\| &\leq \|e_h^n p_h^n - e^n p^n\| + \|e^n e^n - e_h^n e_h^n\| \\ &\quad + \|e_h^n N - e^n N\| \\ &= W_1 + W_2 + W_3. \end{aligned}$$

From (29), we can determine the following:

$$\begin{aligned}
W_1 &\leq \|e_h^n(p_h^n - R_h p^n)\| + \|(e_h^n - R_h e^n)R_h p^n\| + \|R_h e^n(R_h p^n - p^n)\| \\
&\quad + \|(R_h e^n - e^n)p^n\| \\
&\leq \|e_h^n\|_{0,\infty} \|p_h^n - R_h p^n\| + \|R_h p^n\|_{0,\infty} \|e_h^n - R_h e^n\| \\
&\quad + \|R_h e^n\|_{0,\infty} \|R_h p^n - p^n\| + \|p^n\|_{0,\infty} \|R_h e^n - e^n\| \\
&\leq C(\|\zeta_p^n\| + \|\zeta_e^n\| + h_c^{l+1}), \\
W_2 &\leq \|(e^n - R_h e^n)e^n\| + \|R_h e^n(e^n - e_h^n)\| + \|(R_h e^n - e_h^n)e_h^n\| \\
&\leq C(\|\zeta_e^n\| + h_c^{l+1}), \\
W_3 &\leq C(\|e_h^n - R_h e^n\| + \|R_h e^n - e^n\|) \leq C(\|\zeta_e^n\| + h_c^{l+1}).
\end{aligned}$$

Thus, we have

$$\begin{aligned}
|F_8| &\leq C \sum_{n=1}^m \|e_h^n(p_h^n - e_h^n + N) - e^n(p^n - e^n + N)\| \|\partial_t \zeta_e^n\| \Delta t \\
&\leq C(\varepsilon) \left(\sum_{n=1}^m (\|\zeta_e^n\|^2 + \|\zeta_p^n\|^2) \Delta t + h_c^{2l+2} \right) + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \quad (47)
\end{aligned}$$

Combining (39) with (40)–(47) and noting that $e_h^0 = R_h e^0$ and $p_h^0 = R_h p^0$, we have

$$\begin{aligned}
\sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t + \|\nabla \zeta_e^m\|^2 &\leq C(\varepsilon) \left(h_c^{2l} + h_\psi^{2k+2} + (\Delta t)^2 + \sum_{n=1}^m (\|\zeta_e^n\|_1^2 + \|\zeta_p^n\|^2) \Delta t \right) \\
&\quad + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \quad (48)
\end{aligned}$$

To obtain the H^1 norm of $\nabla \zeta_e^m$, we add $\|\zeta_e^m\|^2$ to the above equation. Note that

$$\begin{aligned}
\|\zeta_e^n\|^2 - \|\zeta_e^{n-1}\|^2 &= (\zeta_e^n + \zeta_e^{n-1}, \zeta_e^n - \zeta_e^{n-1}) \\
&= (\zeta_e^n - \zeta_e^{n-1}, \zeta_e^n - \zeta_e^{n-1}) + 2(\zeta_e^{n-1}, \zeta_e^n - \zeta_e^{n-1}) \\
&= \left\| \frac{\zeta_e^n - \zeta_e^{n-1}}{\Delta t} \right\|^2 (\Delta t)^2 + 2 \left(\zeta_e^{n-1}, \frac{\zeta_e^n - \zeta_e^{n-1}}{\Delta t} \right) \Delta t \\
&\leq C(\varepsilon) \|\zeta_e^{n-1}\|^2 \Delta t + (\Delta t + \varepsilon) \left\| \frac{\zeta_e^n - \zeta_e^{n-1}}{\Delta t} \right\|^2 \Delta t.
\end{aligned}$$

The both sides of the above inequality are sum from $n = 1$ to m , then we have

$$\|\zeta_e^m\|^2 \leq C(\varepsilon) \sum_{n=1}^m \|\zeta_e^n\|^2 \Delta t + (\Delta t + \varepsilon) \sum_{n=1}^m \|\partial_t \zeta_e^n\|^2 \Delta t. \quad (49)$$

Similarly, for the L^2 estimates of $\nabla \zeta_p$ and ζ_p , we find that

$$\begin{aligned}
\sum_{n=1}^m \|\partial_t \zeta_p^n\|^2 \Delta t + \|\nabla \zeta_p^m\|^2 &\leq C(\varepsilon) \left(h_c^{2l} + h_\psi^{2k+2} + (\Delta t)^2 + \sum_{n=1}^m (\|\zeta_p^n\|_1^2 + \|\zeta_e^n\|^2) \Delta t \right) \\
&\quad + \varepsilon \sum_{n=1}^m \|\partial_t \zeta_p^n\|^2 \Delta t, \quad (50)
\end{aligned}$$

$$\|\zeta_p^m\|^2 \leq C(\varepsilon) \sum_{n=1}^m \|\zeta_p^n\|^2 \Delta t + (\Delta t + \varepsilon) \sum_{n=1}^m \|\partial_t \zeta_p^n\|^2 \Delta t. \quad (51)$$

Combining (48)–(51) and selecting sufficiently small values of Δt and ε , we obtain

$$\sum_{n=1}^m (\|\partial_t \zeta_e^n\|^2 + \|\partial_t \zeta_p^n\|^2) \Delta t + \|\zeta_e^m\|_1^2 + \|\zeta_p^m\|_1^2 \leq C \left(h_c^{2l} + h_\psi^{2k+2} + (\Delta t)^2 + \sum_{n=1}^m (\|\zeta_e^n\|_1^2 + \|\zeta_p^n\|_1^2) \Delta t \right),$$

where $C = C(\varepsilon)$ is a constant that depends on ε . An application of the discrete Gronwall Lemma yields the following:

$$\|\zeta_e^m\|_1^2 + \|\zeta_p^m\|_1^2 \leq C(h_c^{2l} + h_\psi^{2k+2} + (\Delta t)^2).$$

Then, for $1 \leq m \leq N$, we determine that

$$\|\zeta_e^m\|_1 \leq C(h_c^l + h_\psi^{k+1} + \Delta t).$$

Similar to the proof process of Theorem 3.4 in [19], we determine that

$$\|\zeta_e^n\|_{1,q} \leq C(h_c^l + h_\psi^{k+1} + \Delta t), \quad 2 < q \leq \infty. \quad (52)$$

We apply a duality argument to estimate $\|e_h^n - R_h e^n\|_{0,q}$ by considering an auxiliary problem: find $\omega \in H_0^1(\Omega)$ such that

$$a(v, \omega) = (\varphi, v), \quad v \in H_0^1(\Omega).$$

This problem is uniquely solvable for $\omega \in L^q(\Omega)$, and

$$\|\omega\|_{2,p} \leq C\|\varphi\|_{0,p}, \quad \varphi \in L^p(\Omega),$$

where $p = q/(q-1) \in [1, 2]$ for $2 \leq q \leq \infty$. If $s = 2q/(q+2)$, applying the Sobolev embedding theorem, we have

$$\|R_h \omega\|_{1,s/(s-1)} \leq C\|\omega\|_{1,s/(s-1)} \leq C\|\omega\|_{2,p} \leq C\|\varphi\|_{0,p}. \quad (53)$$

By Lemma 3.1 of [19] and (53), we have

$$\begin{aligned} (e_h^n - R_h e^n, \varphi) &= a(e_h^n - R_h e^n, \omega) = a(e_h^n - R_h e^n, \omega - R_h \omega) + a(e_h^n - e^n, R_h \omega) \\ &\leq C(\|e_h^n - R_h e^n\|_{1,q} \|\omega - R_h \omega\|_{1,p} + \|e_h^n - e^n\|_{1,2s}^2 \|R_h \omega\|_{1,s/(s-1)}) \\ &\leq C(h_c \|e_h^n - R_h e^n\|_{1,q} + \|e_h^n - e^n\|_{1,2s}^2) \|\varphi\|_{0,p}. \end{aligned}$$

For $q = 2$, since $s = 1$, from (52), we have the following:

$$\begin{aligned} \|e_h^n - R_h e^n\|_{0,q} &\leq C(h_c \|e_h^n - R_h e^n\|_{1,q} + \|e_h^n - e^n\|_{1,2s}^2) \\ &\leq C(h_c \|e_h^n - R_h e^n\|_{1,q} + \|e_h^n - R_h e^n\|_{1,2+\varepsilon}^2 + \|R_h e^n - e^n\|_{1,2+\varepsilon}^2) \\ &\leq C(h_c^{l+1} + h_\psi^{k+1} + \Delta t). \end{aligned}$$

For $2 < q < \infty$, since $2s < q$, we have

$$\begin{aligned} \|e_h^n - R_h e^n\|_{0,q} &\leq C(h_c \|e_h^n - R_h e^n\|_{1,q} + \|e_h^n - R_h e^n\|_{1,q}^2 + \|R_h e^n - e^n\|_{1,q}^2) \\ &\leq C(h_c^{l+1} + h_\psi^{k+1} + \Delta t), \end{aligned}$$

which yields (36). Similarly, we can obtain (37). \square

From Lemmas 3.1 and 3.2, we obtain the following important theorem:

Theorem 3.3. *Let (e^n, p^n) be the solution of (15)–(16) at t^n , and (e_h^n, p_h^n) be the finite element solution of (19)–(20). If the regularity assumptions (A) hold, and the initial functions $e_h^0 = R_h e^0$ and $p_h^0 = R_h p^0$, then for $1 \leq n \leq N$, $2 \leq q < \infty$ and $l, k \geq 1$, we have*

$$\|e_h^n - e^n\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + \Delta t), \quad (54)$$

$$\|p_h^n - p^n\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + \Delta t). \quad (55)$$

3.3. L^q error estimate of mixed finite method. First, it is useful to denote the L^2 projection Q_h as follows. For $\rho \in (L^2(\Omega))^2$,

$$(\rho, \mathbf{v}_h) = (Q_h \rho, \mathbf{v}_h), \quad \forall \mathbf{v}_h \in \mathbf{V}_h. \quad (56)$$

For $\rho \in (W^{k+1,q}(\Omega))^2$, the L^2 projection operator has approximation property [11]:

$$\|\rho - Q_h \rho\|_{0,q} \leq C\|\rho\|_{r,q} h^r, \quad 0 \leq r \leq k+1. \quad (57)$$

Next, the L^q error estimate of the electrostatic potential will be obtained. We obtain the following error equations by subtracting (13) and (14) from (21) and (22), respectively:

$$(R_h \mathbf{u} - \mathbf{u}, \mathbf{v}) - (\nabla \cdot \mathbf{v}, R_h \psi - \psi) = 0, \quad \forall \mathbf{v} \in \mathbf{V}_h, \quad (58)$$

$$(\nabla \cdot (R_h \mathbf{u} - \mathbf{u}), w) = 0, \quad \forall w \in W_h. \quad (59)$$

Let D_h be the L^2 -projection onto the space

$$\bar{\mathbf{V}}_h = \{\mathbf{v} \in \mathbf{V}_h \mid \nabla \cdot \mathbf{v} = 0\}. \quad (60)$$

D_h has the following stability property [7]:

$$\|D_h \mathbf{v}\|_{0,q} \leq C\|\mathbf{v}\|_{0,q}, \quad 2 \leq q < \infty. \quad (61)$$

Lemma 3.4. *If \mathbf{u}^n and $R_h \mathbf{u}^n$ are the solutions of (13)–(14) and (21)–(22), respectively, at $t = t^n$. For $1 \leq n \leq N$, $2 \leq q < \infty$ and $k \geq 1$, we have*

$$\|\mathbf{u}^n - R_h \mathbf{u}^n\|_{0,q} \leq C\|\mathbf{u}^n\|_{k+1,q} h_\psi^{k+1}. \quad (62)$$

Proof. This Lemma can be easily derived from (58) and (60). More details of the proof can be found in [6, Lemma 3.2] and [5, Lemma 4.1]. \square

For (25), if $1/p + 1/q = 1$, we have

$$\begin{aligned} \|\nabla \cdot (\mathbf{u}_h^n - R_h \mathbf{u}^n)\|_{0,q} &= \sup_{w \in W_h} \frac{|(\nabla \cdot (\mathbf{u}_h^n - R_h \mathbf{u}^n), w)|}{\|w\|_{0,p}} \\ &= \sup_{w \in W_h} \frac{|\alpha(p_h^n - p^n - e_h^n + e^n, w)|}{\|w\|_{0,p}} \\ &\leq C(\|e^n - e_h^n\|_{0,q} + \|p^n - p_h^n\|_{0,q}) \\ &\leq C(h_c^{l+1} + h_\psi^{k+1} + \Delta t). \end{aligned} \quad (63)$$

Lastly, we obtain the L^q error estimate of the electric field intensity:

$$\|\mathbf{u}^n - \mathbf{u}_h^n\|_{0,q} \leq \|\mathbf{u}^n - R_h \mathbf{u}^n\|_{0,q} + \|R_h \mathbf{u}^n - \mathbf{u}_h^n\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + \Delta t). \quad (64)$$

4. Two-grid algorithm and error estimate. The two-grid algorithm and its convergence analysis are presented in this section. The fundamental ingredient of the scheme is a new finite element space $\mathbf{V}_H \times W_H \times M_H \times M_H \subset \mathbf{V}_h \times W_h \times M_h \times M_h$ ($h < H < 1$) defined on a coarser quasi-uniform triangulation or rectangulation of Ω . The non-linear equations can be solved by applying the Newton iteration procedure on the fine grid to linearize the non-linear system. The solutions of the original non-linear system will be reduced to the solutions of a small-scale non-linear system on the coarse space and a linear system on the fine space. First, we provide the two-grid algorithm.

Step 1. Solve the non-linear coupled system for $(\mathbf{u}_H^n, \psi_H^n, e_H^n, p_H^n) \in \mathbf{V}_H \times W_H \times M_H \times M_H$ on the coarse grid \mathcal{T}_H :

$$(\mathbf{u}_H^n, \mathbf{v}) - (\nabla \cdot \mathbf{v}, \psi_H^n) = 0, \quad \forall \mathbf{v} \in \mathbf{V}_H, \quad (65)$$

$$(\nabla \cdot \mathbf{u}_H^n, w) = \alpha(p_H^n - e_H^n + N, w), \quad \forall w \in W_H, \quad (66)$$

$$\begin{aligned} & (\partial_{\tau_e} e_H^n, z) + (D_e \nabla e_H^n, \nabla z) - (e_H^n \mathbf{u}_H^n \cdot \nabla \mu_e, z) - \alpha(\mu_e e_H^n (p_H^n - e_H^n + N), z) \\ &= -(R(e_H^n, p_H^n), z), \quad \forall z \in M_H, \end{aligned} \quad (67)$$

$$\begin{aligned} & (\partial_{\tau_p} p_H^n, z) + (D_p \nabla p_H^n, \nabla z) + (p_H^n \mathbf{u}_H^n \cdot \nabla \mu_p, z) + \alpha(\mu_p p_H^n (p_H^n - e_H^n + N), z) \\ &= -(R(e_H^n, p_H^n), z), \quad \forall z \in M_H. \end{aligned} \quad (68)$$

Step 2. Solve the linear coupled system for $(\mathbf{U}_h^n, \Psi_h^n, E_h^n, P_h^n) \in \mathbf{V}_h \times W_h \times M_h \times M_h$ on the fine grid \mathcal{T}_h :

$$(\mathbf{U}_h^n, \mathbf{v}) - (\nabla \cdot \mathbf{v}, \Psi_h^n) = 0, \quad \forall \mathbf{v} \in \mathbf{V}_h, \quad (69)$$

$$(\nabla \cdot \mathbf{U}_h^n, w) = \alpha(P_h^n - E_h^n + N, w), \quad \forall w \in W_h, \quad (70)$$

$$\begin{aligned} & (\partial_{\tau_e} E_h^n, z) + (D_e \nabla E_h^n, \nabla z) - ([e_H^n \mathbf{U}_h^n + (E_h^n - e_H^n) \mathbf{u}_H^n] \cdot \nabla \mu_e, z) \\ & - \alpha(\mu_e [e_H^n (P_h^n - E_h^n + N) + (E_h^n - e_H^n)(p_H^n - e_H^n + N)], z) \\ &= -(\mathcal{R}(E_h^n, P_h^n), z), \quad \forall z \in M_h, \end{aligned} \quad (71)$$

$$\begin{aligned} & (\partial_{\tau_p} P_h^n, z) + (D_p \nabla P_h^n, \nabla z) + ([p_H^n \mathbf{U}_h^n + (P_h^n - p_H^n) \mathbf{u}_H^n] \cdot \nabla \mu_p, z) \\ & + \alpha(\mu_p [p_H^n (P_h^n - E_h^n + N) + (P_h^n - p_H^n)(p_H^n - e_H^n + N)], z) \\ &= -(\mathcal{R}(E_h^n, P_h^n), z), \quad \forall z \in M_h, \end{aligned} \quad (72)$$

where $\mathcal{R}(E_h^n, P_h^n) = R(e_H^n, p_H^n) + R_e(e_H^n, p_H^n)(E_h^n - e_H^n) + R_p(e_H^n, p_H^n)(P_h^n - p_H^n)$.

Next, we present an error estimation analysis of the exact solutions $(\mathbf{u}^n, \psi^n, e^n, p^n)$ and two-grid solutions $(\mathbf{U}_h^n, \Psi_h^n, E_h^n, P_h^n)$. We note that $(\mathbf{U}_h^n, \Psi_h^n)$ are the two-grid solutions defined in (69) and (70). Using (23), (26), and triangle inequality, we can analyze the electrostatic potential and electric field intensity:

$$\|\mathbf{u}^n - \mathbf{U}_h^n\|_V + \|\psi^n - \Psi_h^n\|_W \leq C(h_\psi^{k+1} + \|e^n - E_h^n\| + \|p^n - P_h^n\|). \quad (73)$$

Next, we prove $\|e^n - E_h^n\|_{0,q}$ and $\|p^n - P_h^n\|_{0,q}$. The elliptic projection will be used as an intermediate variable to assist this proof, and the main results are as follows:

Lemma 4.1. *Let $(R_h e^n, R_h p^n)$ be the elliptic projection solution of (27)–(28) at $t = t^n$, (E_h^n, P_h^n) be the two-grid solution of (71)–(72). If we choose $E_h^0 = R_h e^0$ and $P_h^0 = R_h p^0$, the regularity assumptions (A) hold, then for $1 \leq n \leq N$, $2 \leq q < \infty$*

and $l, k \geq 1$, we have

$$\|R_h e^n - E_h^n\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + H_c^{2l+2} + H_\psi^{2k+2} + \Delta t), \quad (74)$$

$$\|R_h p^n - P_h^n\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + H_c^{2l+2} + H_\psi^{2k+2} + \Delta t). \quad (75)$$

Proof. We subtract (15) and (27) from (71) at $t = t^n$ to obtain the following error equation:

$$\begin{aligned} & (\partial_{\tau_e} E_h^n, z) - (\phi_e^n \frac{\partial e^n}{\partial \tau_e}, z) + (D_e \nabla(E_h^n - R_h e^n), \nabla z) \\ &= ([e_H^n \mathbf{U}_h^n + (E_h^n - e_H^n) \mathbf{u}_H^n - e^n \mathbf{u}^n] \cdot \nabla \mu_e, z) + \alpha(\mu_e [e_H^n (P_h^n - E_h^n + N) \\ & \quad + (E_h^n - e_H^n)(p_H^n - e_H^n + N) - e^n(p^n - e^n + N)], z) \\ & \quad + (R(e^n, p^n) - \mathcal{R}(E_h^n, P_h^n), z) + \lambda_e(R_h e^n - e^n, z), \quad \forall z \in M_h. \end{aligned} \quad (76)$$

We let $\eta_e^n = E_h^n - R_h e^n$ and $\eta_p^n = P_h^n - R_h p^n$ and select $z = \eta_e^n - \eta_e^{n-1} = \partial_t \eta_e^n \Delta t$. Summing over $1 \leq n \leq m$, from (76), we have

$$\sum_{n=1}^m (\partial_t \eta_e^n, \partial_t \eta_e^n) \Delta t + \frac{1}{2} (D_e \nabla \eta_e^m, \nabla \eta_e^m) - \frac{1}{2} (D_e \nabla \eta_e^0, \nabla \eta_e^0) \leq \sum_{i=1}^8 K_i, \quad (77)$$

where

$$\begin{aligned} K_1 &= \sum_{n=1}^m \left(R(e^n, p^n) - \mathcal{R}(E_h^n, P_h^n), \partial_t \eta_e^n \right) \Delta t, & K_2 &= \sum_{n=1}^m \left(\frac{\xi_e^n - \xi_e^{n-1}}{\Delta t}, \partial_t \eta_e^n \right) \Delta t, \\ K_3 &= \sum_{n=1}^m \left(\frac{\xi_e^{n-1} - \hat{\xi}_e^{n-1}}{\Delta t}, \partial_t \eta_e^n \right) \Delta t, & K_4 &= \sum_{n=1}^m \left(\frac{\hat{\eta}_e^{n-1} - \eta_e^{n-1}}{\Delta t}, \partial_t \eta_e^n \right) \Delta t, \\ K_5 &= \sum_{n=1}^m \left(\phi_e^n \frac{\partial e^n}{\partial \tau_e} - \frac{e^n - \hat{e}^{n-1}}{\Delta t}, \partial_t \eta_e^n \right) \Delta t, & K_6 &= - \sum_{n=1}^m \lambda_e(\xi_e^n, \partial_t \eta_e^n) \Delta t, \\ K_7 &= \sum_{n=1}^m \left([e_H^n \mathbf{U}_h^n + (E_h^n - e_H^n) \mathbf{u}_H^n - e^n \mathbf{u}^n] \cdot \nabla \mu_e, \partial_t \eta_e^n \right) \Delta t, \\ K_8 &= \sum_{n=1}^m \alpha \left(\mu_e [e_H^n (P_h^n - E_h^n + N) + (E_h^n - e_H^n)(p_H^n - e_H^n + N) \right. \\ & \quad \left. - e^n(p^n - e^n + N)], \partial_t \eta_e^n \right) \Delta t. \end{aligned}$$

Now we estimate each term on the right hand of (77) as follows. First, using a second-order Taylor expansion at point (e_H^n, p_H^n) for $R(e^n, p^n)$, (29), (54) and (55), we have

$$\begin{aligned} |K_1| &\leq \sum_{n=1}^m \| (R_e(e_H^n, p_H^n)(e^n - E_h^n) + R_p(e_H^n, p_H^n)(p^n - P_h^n) \\ & \quad + \frac{1}{2} R_{ee}(e^*, p^*)(e^n - e_H^n)^2 + R_{ep}(e^*, p^*)(e^n - e_H^n)(p^n - p_H^n) \\ & \quad + \frac{1}{2} R_{pp}(e^*, p^*)(p^n - p_H^n)^2 \| \|\partial_t \eta_e^n\| \Delta t \\ &\leq C \sum_{n=1}^m (\|e^n - E_h^n\| + \|p^n - P_h^n\| + \|e^n - e_H^n\|_{0,4}^2 + \|e^n - e_H^n\|_{0,4} \|p^n - p_H^n\|_{0,4}) \end{aligned}$$

$$\begin{aligned}
& + \|p^n - p_H^n\|_{0,4}^2 \|\partial_t \eta_e^n\| \Delta t \\
& \leq C \left(h_c^{2l+2} + H_c^{4l+4} + H_\psi^{4k+4} + (\Delta t)^4 + \sum_{n=1}^m (\|\eta_e^n\|^2 + \|\eta_p^n\|^2) \Delta t \right) \\
& + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t,
\end{aligned} \tag{78}$$

where e^* is a point between e^n and e_H^n , p^* is a point between p^n and p_H^n .

Similar to the proof process of Lemma 3.2, we give the following error estimations directly,

$$|K_2| \leq C h_c^{2l+2} + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t, \tag{79}$$

$$|K_3| \leq C h_c^{2l} + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t, \tag{80}$$

$$|K_4| \leq C \sum_{n=1}^m \|\nabla \eta_e^{n-1}\|^2 \Delta t + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t, \tag{81}$$

$$|K_5| \leq C (\Delta t)^2 \left\| \frac{\partial^2 e}{\partial \tau_e^2} \right\|_{L^2(J; L^2(\Omega))}^2 + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t, \tag{82}$$

$$|K_6| \leq C h_c^{2l+2} + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \tag{83}$$

For K_7 , we have

$$\begin{aligned}
e_H^n \mathbf{U}_h^n + (E_h^n - e_H^n) \mathbf{u}_H^n - e^n \mathbf{u}^n &= e_H^n (\mathbf{U}_h^n - \mathbf{u}^n) + (e_H^n - E_h^n) (\mathbf{u}^n - \mathbf{u}_H^n) \\
&+ (E_h^n - e^n) \mathbf{u}^n \\
&= I_1 + I_2 + I_3.
\end{aligned}$$

Using (73) and (29), we have

$$\begin{aligned}
\left| \sum_{n=1}^m (I_1, \partial_t \eta_e^n) \Delta t \right| &\leq C \sum_{n=1}^m \|\mathbf{u}^n - \mathbf{U}_h^n\| \|\partial_t \eta_e^n\| \Delta t \\
&\leq C \left(\sum_{n=1}^m (\|\eta_e^n\|^2 + \|\eta_p^n\|^2) \Delta t + h_c^{2l+2} + h_\psi^{2k+2} \right) + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t.
\end{aligned} \tag{84}$$

Using (64), (54), and (31), we have

$$\begin{aligned}
\left| \sum_{n=1}^m (I_2, \partial_t \eta_e^n) \Delta t \right| &= \left| \sum_{n=1}^m ((e_H^n - e^n) (\mathbf{u}^n - \mathbf{u}_H^n) + (e^n - R_h e^n) (\mathbf{u}^n - \mathbf{u}_H^n) \right. \\
&\quad \left. + (R_h e^n - E_h^n) (\mathbf{u}^n - \mathbf{u}_H^n), \partial_t \eta_e^n) \Delta t \right| \\
&\leq \sum_{n=1}^m (\|e_H^n - e^n\|_{0,4} \|\mathbf{u}^n - \mathbf{u}_H^n\|_{0,4} + \|e^n - R_h e^n\|_{0,4} \|\mathbf{u}^n - \mathbf{u}_H^n\|_{0,4} \\
&\quad + \|\mathbf{u}^n - \mathbf{u}_H^n\|_{0,\infty} \|R_h e^n - E_h^n\|) \|\partial_t \eta_e^n\| \Delta t
\end{aligned}$$

$$\begin{aligned} &\leq C \left(H_c^{4l+4} + H_\psi^{4k+4} + h_c^{4l+4} + (\Delta t)^4 + \sum_{n=1}^m \|\eta_e^n\|^2 \Delta t \right) \\ &\quad + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t, \end{aligned} \quad (85)$$

$$\begin{aligned} \left| \sum_{n=1}^m (I_3, \partial_t \eta_e^n) \Delta t \right| &\leq C \sum_{n=1}^m (\|E_h^n - R_h e^n\| + \|R_h e^n - e^n\|) \|\partial_t \eta_e^n\| \Delta t \\ &\leq C \left(\sum_{n=1}^m \|\eta_e^n\|^2 \Delta t + h_c^{2l+2} \right) + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \end{aligned} \quad (86)$$

From (84)–(86), we obtain

$$\begin{aligned} |K_7| &\leq C \left(\sum_{n=1}^m (\|\eta_e^n\|^2 + \|\eta_p^n\|^2) \Delta t + h_c^{2l+2} + h_\psi^{2k+2} + H_c^{4l+4} + H_\psi^{4k+4} + (\Delta t)^4 \right) \\ &\quad + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \end{aligned} \quad (87)$$

For K_8 , we have

$$\begin{aligned} &e_H^n (P_h^n - E_h^n + N) + (E_h^n - e_H^n) (p_H^n - e_H^n + N) - e^n (p^n - e^n + N) \\ &= (E_h^n - e^n) (p^n - e^n + N) + (e_H^n - E_h^n) (p^n - p_H^n + e_H^n - e^n) \\ &\quad - e_H^n (p^n - P_h^n + E_h^n - e^n) \\ &= J_1 + J_2 + J_3. \end{aligned}$$

Related to J_1 , we have

$$\begin{aligned} \left| \sum_{n=1}^m (J_1, \partial_t \eta_e^n) \Delta t \right| &\leq C \sum_{n=1}^m \|E_h^n - e^n\| \|\partial_t \eta_e^n\| \Delta t \\ &\leq C \left(\sum_{n=1}^m \|\eta_e^n\|^2 \Delta t + h_c^{2l+2} \right) + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \end{aligned} \quad (88)$$

Related to J_2 , we have

$$\begin{aligned} \left| \sum_{n=1}^m (J_2, \partial_t \eta_e^n) \Delta t \right| &= \left| \sum_{n=1}^m ((e_H^n - E_h^n) (p^n - p_H^n) + (e_H^n - E_h^n) (e_H^n - e^n), \partial_t \eta_e^n) \Delta t \right| \\ &= \left| \sum_{n=1}^m (J_{21} + J_{22}, \partial_t \eta_e^n) \Delta t \right|. \end{aligned}$$

Using (54), (55), and (31), we have

$$\begin{aligned} \left| \sum_{n=1}^m (J_{21}, \partial_t \eta_e^n) \Delta t \right| &= \left| \sum_{n=1}^m ((e_H^n - e^n) (p^n - p_H^n) + (e^n - R_h e^n) (p^n - p_H^n) \right. \\ &\quad \left. + (R_h e^n - E_h^n) (p^n - p_H^n), \partial_t \eta_e^n) \Delta t \right| \\ &\leq \sum_{n=1}^m (\|e_H^n - e^n\|_{0,4} \|p^n - p_H^n\|_{0,4} + \|e^n - R_h e^n\|_{0,4} \|p^n - p_H^n\|_{0,4} \\ &\quad + \|p^n - p_H^n\|_{0,\infty} \|R_h e^n - E_h^n\|) \|\partial_t \eta_e^n\| \Delta t \end{aligned}$$

$$\begin{aligned}
&\leq C \left(H_c^{4l+4} + H_\psi^{4k+4} + h_c^{4l+4} + (\Delta t)^4 + \sum_{n=1}^m \|\eta_e^n\|^2 \Delta t \right) \\
&\quad + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \tag{89}
\end{aligned}$$

Similar to J_{21} , we have the same estimation of J_{22} . Finally, for J_3 we have

$$\begin{aligned}
\left| \sum_{n=1}^m (J_3, \partial_t \eta_e^n) \Delta t \right| &\leq C \sum_{n=1}^m (\|p^n - P_h^n\| + \|E_h^n - e^n\|) \|\partial_t \eta_e^n\| \Delta t \\
&\leq C \left(\sum_{n=1}^m (\|\eta_e^n\|^2 + \|\eta_p^n\|^2) \Delta t + h_c^{2l+2} \right) + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \tag{90}
\end{aligned}$$

From (88)–(90), we obtain

$$\begin{aligned}
|K_8| &\leq C \left(\sum_{n=1}^m (\|\eta_e^n\|^2 + \|\eta_p^n\|^2) \Delta t + h_c^{2l+2} + H_c^{4l+4} + H_\psi^{4k+4} + (\Delta t)^4 \right) \\
&\quad + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \tag{91}
\end{aligned}$$

Combining (77) with estimates (78)–(83), (87) and (91), and noting that $E_h^0 = R_h e^0$ and $P_h^0 = R_h p^0$, we have

$$\begin{aligned}
\sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t + \|\nabla \eta_e^m\|^2 &\leq C \left(h_c^{2l} + h_\psi^{2k+2} + H_c^{4l+4} + H_\psi^{4k+4} + (\Delta t)^2 \right. \\
&\quad \left. + \sum_{n=1}^m (\|\eta_e^n\|_1^2 + \|\eta_p^n\|^2) \Delta t \right) + \varepsilon \sum_{n=1}^m \|\partial_t \eta_e^n\|^2 \Delta t. \tag{92}
\end{aligned}$$

Similar to the proof process of Lemma 3.2, we determine that

$$\|\eta_e^m\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + H_c^{2l+2} + H_\psi^{2k+2} + \Delta t), \tag{93}$$

which yields (74). Similarly, we can obtain (75). \square

Using the triangle inequality, (31), (32), and Lemma 4.1, we have the following results:

Theorem 4.2. *Let (e^n, p^n) be the solution of (15)–(16) at $t = t^n$, and (E_h^n, P_h^n) be the two-grid solution of (71)–(72). If the regularity assumptions (A) hold, and the initial functions $E_h^0 = R_h e^0$ and $P_h^0 = R_h p^0$, then for $1 \leq n \leq N$, $2 \leq q < \infty$ and $l, k \geq 1$, we have*

$$\|e^n - E_h^n\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + H_c^{2l+2} + H_\psi^{2k+2} + \Delta t), \tag{94}$$

$$\|p^n - P_h^n\|_{0,q} \leq C(h_c^{l+1} + h_\psi^{k+1} + H_c^{2l+2} + H_\psi^{2k+2} + \Delta t). \tag{95}$$

Lastly, from Theorem 4.2 and (73), we obtain

Theorem 4.3. *Let (ψ^n, \mathbf{u}^n) be the solution of (13)–(14) at $t = t^n$, and $(\Psi_h^n, \mathbf{U}_h^n)$ be the two-grid solution of (69)–(70). If the regularity assumptions (A) hold, and the initial functions $E_h^0 = R_h e^0$ and $P_h^0 = R_h p^0$, then for $1 \leq n \leq N$ and $l, k \geq 1$, we have*

$$\|\mathbf{u}^n - \mathbf{U}_h^n\|_{\mathbf{V}} + \|\psi^n - \Psi_h^n\|_W \leq C(h_c^{l+1} + h_\psi^{k+1} + H_c^{2l+2} + H_\psi^{2k+2} + \Delta t). \tag{96}$$

5. Numerical experiment. In this section, the numerical experiment is presented to illustrate the efficiency of the two-grid method for solving the semiconductor device problem in Section 4.

We consider the following equations with Dirichlet boundary condition:

$$-\Delta\psi = p - e, \quad (97)$$

$$\frac{\partial e}{\partial t} - \Delta e + \nabla \cdot (e \nabla \psi) = f_1, \quad (98)$$

$$\frac{\partial p}{\partial t} - \Delta p - \nabla \cdot (p \nabla \psi) = f_2, \quad (99)$$

where $\Omega = (0, 1)^2$, $t \in [0, T]$. We take the exact solutions of (97)–(99) are

$$\psi = \exp(t) \sin(\pi x_1) \sin(\pi x_2) - t^3 \sin(2\pi x_1) \sin(2\pi x_2),$$

$$e = 8\pi^2 t^3 \sin(2\pi x_1) \sin(2\pi x_2),$$

$$p = 2\pi^2 \exp(t) \sin(\pi x_1) \sin(\pi x_2).$$

The right hand sides f_1 and f_2 are determined by the above exact solutions.

We use piecewise constant for ψ , the lowest Raviart–Thomas element for \mathbf{u} and piecewise linear continuous function for e, p . We select the time step $\tau = 1.0e - 2$ and $T = 1$. For the sake of simplicity, we assume $h_\psi = h_c = h$, $H_\psi = H_c = H$. The exact solutions e^n, p^n, ψ^n , the characteristics finite element and the mixed finite element method solutions e_h^n, p_h^n, ψ_h^n and the two-grid method solutions E_h^n, P_h^n, Ψ_h^n are shown in Figs.1–9. To compare these pictures, we can see that the solutions of finite element method and two-grid method are identical with the exact solutions. From Figs.10–13, we can observe that the convergence rate of the error for $\|e^n - e_h^n\|$, $\|p^n - p_h^n\|$, $\|\psi^n - \psi_h^n\|$, and $\|\mathbf{u}^n - \mathbf{u}_h^n\|$, respectively. In Tables 1–3, we present the numerical results for error estimates and CPU time cost of the finite element method and the two-grid method. As shown in Tables 1–3, we can know that when the coarse grid and the fine grid satisfy $H = h^{\frac{1}{2}}$, the two-grid method achieves the same accuracy as the finite element method but requires less time.

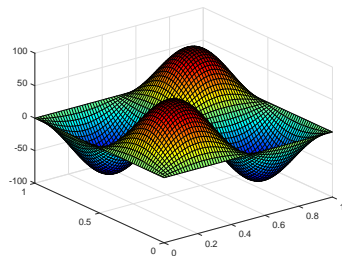


FIGURE 1. The exact solution e^n , $h = 1/64$, $n = 100$

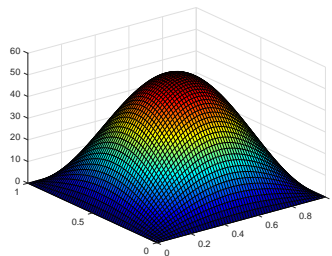


FIGURE 2. The exact solution p^n , $h = 1/64$, $n = 100$

6. Conclusion. This paper has presented a two-grid algorithm for coupled semiconductor device equations discretized by the mixed finite element method and the characteristics finite element method. The fundamental idea of the two-grid

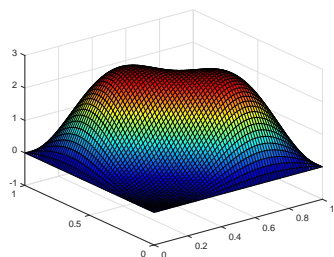


FIGURE 3. The exact solution ψ^n , $h = 1/64$, $n = 100$

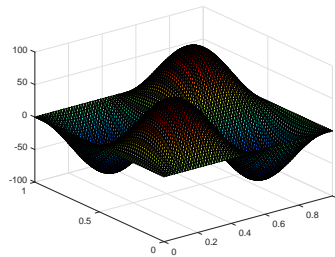


FIGURE 4. Finite element solution e_h^n , $h = 1/64$, $n = 100$

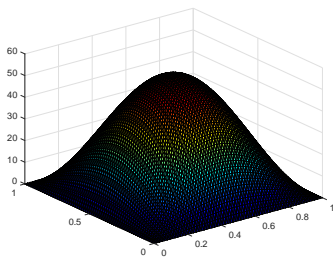


FIGURE 5. Finite element solution p_h^n , $h = 1/64$, $n = 100$

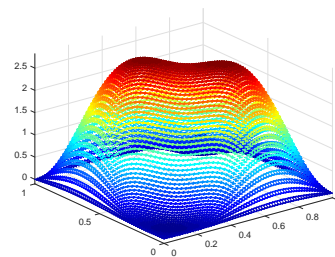


FIGURE 6. Finite element solution ψ_h^n , $h = 1/64$, $n = 100$

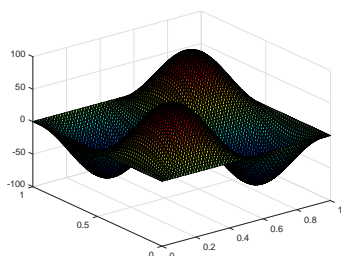


FIGURE 7. Two-grid solution E_h^n , $H = 1/8$, $h = 1/64$, $n = 100$

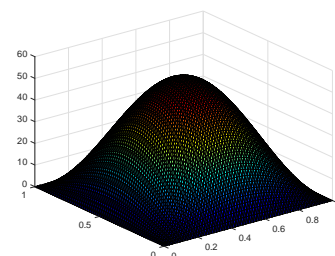


FIGURE 8. Two-grid solution P_h^n , $H = 1/8$, $h = 1/64$, $n = 100$

method is that we can solve non-linear equations by applying the Newton iteration procedure on the fine grid to linearize the non-linear system. It was shown that the two-grid method still achieves asymptotically optimal approximations as long as a mesh size between those of coarse and fine grids satisfies $H = O(h^{1/2})$. From

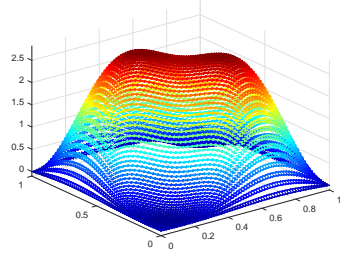


FIGURE 9. Two-grid solution Ψ_h^n , $H = 1/8$, $h = 1/64$, $n = 100$

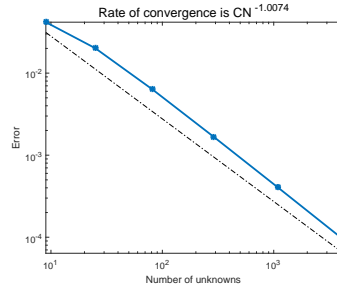


FIGURE 10. Order of finite element solution e_h^n , $n = 100$

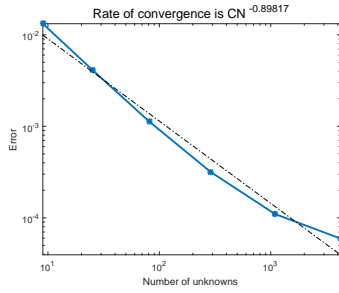


FIGURE 11. Order of finite element solution p_h^n , $n = 100$

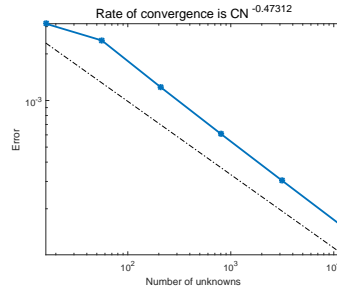


FIGURE 12. Order of finite element solution u_h^n , $n = 100$

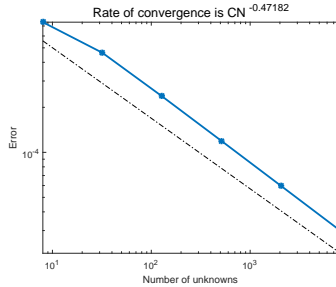


FIGURE 13. Order of finite element solution ψ_h^n , $n = 100$

TABLE 1. Error and CPU time of the finite element method for $n = 100$

h	$\ e^n - e_h^n\ $	$\ p^n - p_h^n\ $	$\ \psi^n - \psi_h^n\ $	$\ u^n - u_h^n\ $	CPU time
$\frac{1}{4}$	2.0125e-2	4.1448e-3	4.6324e-4	2.4411e-3	0.4850s
$\frac{1}{8}$	6.3665e-3	1.1304e-3	2.3741e-4	1.2207e-3	1.0107s
$\frac{1}{16}$	1.6748e-3	3.1703e-4	1.1935e-4	6.0937e-4	3.4394s
$\frac{1}{32}$	4.0476e-4	1.1037e-4	5.9754e-5	3.0453e-4	15.1790s
$\frac{1}{64}$	9.3634e-5	5.9437e-5	2.9886e-5	1.5224e-4	74.9759s

TABLE 2. Error and CPU time of the two-grid method for $n = 100$, $H = \frac{1}{8}$ with different $h = \frac{1}{16}, \frac{1}{32}, \frac{1}{64}$

H	h	$\ e^n - E_h^n\ $	$\ p^n - P_h^n\ $	$\ \psi^n - \Psi_h^n\ $	$\ u^n - U_h^n\ $	CPU time
$\frac{1}{8}$	$\frac{1}{16}$	1.6698e-3	3.3035e-4	1.1935e-4	6.0937e-4	1.0793s
$\frac{1}{8}$	$\frac{1}{32}$	4.0302e-4	1.1523e-4	5.9754e-5	3.0453e-4	4.1308s
$\frac{1}{8}$	$\frac{1}{64}$	9.7872e-5	6.4727e-5	2.9886e-5	1.5224e-4	20.4816s

TABLE 3. Error and CPU time of the two-grid method for $n = 100$, and $h = H^2 = \frac{1}{4}, \frac{1}{16}, \frac{1}{64}$

H	h	$\ e^n - E_h^n\ $	$\ p^n - P_h^n\ $	$\ \psi^n - \Psi_h^n\ $	$\ u^n - U_h^n\ $	CPU time
$\frac{1}{2}$	$\frac{1}{4}$	2.0132e-2	4.1526e-3	4.6324e-4	2.4411e-3	0.1774s
$\frac{1}{4}$	$\frac{1}{16}$	1.6698e-3	3.3035e-4	1.1935e-4	6.0937e-4	1.0310s
$\frac{1}{8}$	$\frac{1}{64}$	9.7872e-5	6.4727e-5	2.9886e-5	1.5224e-4	20.4816s

the numerical experiment, we can find that less time will be required for the two-grid algorithm since only a small-scale non-linear problem must be solved. Hence, the two-grid method is an effective method for solving the semiconductor device problem. In our future work, we will consider more complicated two-grid algorithms for the semiconductor device problem by the mixed finite element method of characteristics.

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REFERENCES

- [1] R. E. Bank, W. M. Coughran, W. Fichtner, E. H. Grosse, D. J. Rose and R. K. Smith, *Transient simulation of silicon devices and circuits*, *IEEE Trans. Computer-Aided Design of Integrated Circuits and Systems*, **4** (1985), 436–451.
- [2] S. C. Brenner and L. Ridgway Scott, *The Mathematical Theory of Finite Element Methods*, Texts in Applied Mathematics, 15, Springer, New York, 2008.
- [3] F. Brezzi, *On the existence, uniqueness and approximation of saddle-point problems arising from Lagrangian multipliers*, *Rev. Française Automat. Informat. Recherche Opérationnelle Sér. Rouge*, **8** (1974), 129–151.
- [4] C. Chen, M. Yang and C. Bi, *Two-grid methods for finite volume element approximations of nonlinear parabolic equations*, *J. Comput. Appl. Math.*, **228** (2009), 123–132.
- [5] Y. Chen and H. Hu, *Two-grid method for miscible displacement problem by mixed finite element methods and mixed finite element method of characteristics*, *Commun. Comput. Phys.*, **19** (2016), 1503–1528.
- [6] Y. Chen, Y. Huang and D. Yu, *A two-grid method for expanded mixed finite-element solution of semilinear reaction-diffusion equations*, *Internat. J. Numer. Methods Engrg.*, **57** (2003), 193–209.
- [7] Z. Chen, *Expanded mixed element methods for linear second-order elliptic problems. I*, *RAIRO Modél. Math. Anal. Numér.*, **32** (1998), 479–499.
- [8] P. G. Ciarlet, *The Finite Element Method for Elliptic Problems*, Studies in Mathematics and its Applications, 4, North-Holland Publishing Co., Amsterdam-New York-Oxford, 1978.
- [9] X. Dai and X. Cheng, *A two-grid method based on Newton iteration for the Navier–Stokes equations*, *J. Comput. Appl. Math.*, **220** (2008), 566–573.
- [10] C. N. Dawson, M. F. Wheeler and C. S. Woodward, *A two-grid finite difference scheme for nonlinear parabolic equations*, *SIAM J. Numer. Anal.*, **35** (1998), 435–452.

- [11] J. Douglas Jr. and J. E. Roberts, [Global estimates for mixed methods for second order elliptic equations](#), *Math. Comp.*, **44** (1985), 39–52.
- [12] J. Douglas Jr. and T. F. Russell, [Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures](#), *SIAM J. Numer. Anal.*, **19** (1982), 871–885.
- [13] J. Douglas Jr. and Y. Yuan, Finite difference methods for the transient behavior of a semiconductor device, *Mat. Apl. Comput.*, **6** (1987), 25–37.
- [14] H. K. Gummel, [A self-consistent iterative scheme for one-dimensional steady-state transistor calculations](#), *IEEE Trans. Electron Devices*, **11** (1964), 455–465.
- [15] T. I. Seidmann, [Time-dependent solutions of a nonlinear system arising in semiconductor theory. II. Boundaries and periodicity](#), *Nonlinear Anal.*, **10** (1986), 491–502.
- [16] Y. Wang, Y. Chen, Y. Huang and Y. Liu, [Two-grid methods for semi-linear elliptic interface problems by immersed finite element methods](#), *Appl. Math. Mech. (English Ed.)*, **40** (2019), 1657–1676.
- [17] M. F. Wheeler, [A priori \$L_2\$ error estimates for Galerkin approximations to parabolic partial differential equations](#), *SIAM J. Numer. Anal.*, **10** (1973), 723–759.
- [18] J. Xu, [A novel two-grid method for semilinear equations](#), *SIAM J. Sci. Comput.*, **15** (1994), 231–237.
- [19] J. Xu, [Two-grid discretization techniques for linear and nonlinear PDEs](#), *SIAM J. Numer. Anal.*, **33** (1996), 1759–1777.
- [20] C. Xu and T. Hou, [Superclose analysis of a two-grid finite element scheme for semilinear parabolic integro-differential equations](#), *Electron. Res. Arch.*, **28** (2020), 897–910.
- [21] Q. Yang, [A modified upwind finite volume scheme for semiconductor devices](#), *J. Systems Sci. Math. Sci.*, **28** (2008), 725–738.
- [22] Q. Yang and Y. Yuan, [An approximation of semiconductor device by mixed finite element method and characteristics-mixed finite element method](#), *Appl. Math. Comput.*, **225** (2013), 407–424.
- [23] J. Yu, H. Zheng, F. Shi and R. Zhao, [Two-grid finite element method for the stabilization of mixed Stokes-Darcy model](#), *Discrete Contin. Dyn. Syst. Ser. B*, **24** (2019), 387–402.
- [24] Y. Yuan, Finite difference method and analysis for three-dimensional semiconductor device of heat conduction, *Sci. China Ser. A*, **39** (1996), 1140–1151.
- [25] Y. R. Yuan, A mixed finite element method for the transient behavior of a semiconductor device, *Gaoxiao Yingyong Shuxue Xuebao*, **7** (1992), 452–463.
- [26] Y. R. Yuan, Characteristic finite element method and analysis for numerical simulation of semiconductor devices, *Acta Math. Sci. (Chinese)*, **13** (1993), 241–251.
- [27] M. Zlámal, [Finite element solution of the fundamental equations of semiconductor devices. I](#), *Math. Comp.*, **46** (1986), 27–43.

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