Journal of Mathematics Research; Vol. 10, No. 3; June 2018
ISSN 1916-9795 E-ISSN 1916-9809
Published by Canadian Center of Science and Education

A Modified Characteristics-mixed Finite Element for Semiconductor Device of Heat Conduction and Numerical Analysis

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Received: February 28, 2018 Accepted: March 15, 2018 Online Published: May 9, 2018

doi:10.5539/jmr.v10n3p97 URL: https://doi.org/10.5539/jmr.v10n3p97

Abstract

Numerical simulation of a three-dimensional semiconductor device of heat conduction is a fundamental problem in modern information science. The mathematical model is formulated by a nonlinear system of initial-boundary problem, which is interpreted by four partial differential equations: an elliptic equation for electrostatic potential, two convection-diffusion equations for electron concentration and hole concentration, a heat conduction equation for temperature. The electrostatic potential appears within the latter three equations, and the electric field strength controls the concentrations and the temperature. The electric field potential is solved by a mixed finite element method, and the electric field strength is obtained simultaneously. The first order of the accuracy is improved for the latter. The concentrations and temperature are computed by the characteristics-finite element method, where the characteristic approximation is adopted for the hyperbolic term and finite element method is use to treat the diffusion. The composite computational scheme can solve the convection-dominated diffusion equations well because it can cancel numerical dispersion and nonphysical oscillation. The temperature is computed by finite element method, and an interesting simulation tool is proposed for solving semiconductor device problem numerically. By using the technique of a priori estimates of differential equations, an optimal order error estimates is obtained. A theoretical work is shown for numerical simulation of information science, and the actual problem is solved well.

Keywords: three-dimensional semiconductor device, mixed finite element, characteristics-finite element, optimal error estimates, numerical analysis

1. Introduction

In this paper we discuss numerical simulation of a three-dimensional semiconductor device of heat conduction, a fundamental problem in information science. Its mathematical model is formulated by four nonlinear partial differential equations: 1) an elliptic equation for electric potential, 2) a convection-diffusion equation for electron concentration, 3) a convection-diffusion equation for hole concentration, 4) a heat conduction equation for temperature. The electric potential appears within the latter three equations, and the electric field strength controls the concentrations and the temperature. The nonlinear partial differential system with initial-boundary conditions on a three-dimensional domain Ω is defined as follows (Bank, Coughran, Fichtner, Grosse, Rose & Smith, 1985; Jerome, 1994; Lou, 1995; Yuan, 1996),

$$-\Delta\psi = \alpha(p - e + N(X)), \quad X = (x, y, z)^T \in \Omega, \quad t \in J = (0, \bar{T}], \tag{1}$$

$$\frac{\partial e}{\partial t} = \nabla \cdot [D_e(X)\nabla e - \mu_e(X)e\nabla\psi] - R_1(e, p, T), \quad (X, t) \in \Omega \times J, \tag{2}$$

$$\frac{\partial p}{\partial t} = \nabla \cdot \left[D_p(X)\nabla p + \mu_p(X)p\nabla\psi\right] - R_2(e, p, T), \quad (X, t) \in \Omega \times J, \tag{3}$$

$$\rho\frac{\partial T}{\partial t} - \Delta T = \left\{(D_p(X)\nabla p + \mu_p(X)p\nabla\psi) - (D_e(X)\nabla e - \mu_e(X)e\nabla\psi)\right\} \cdot \nabla\psi, \quad (X, t) \in \Omega \times J. \tag{4}$$

The electric potential, electron concentration, hole concentration and temperature are the objective functions, denoted by ψ, e, p and T, respectively. All the coefficients of (1)-(4) are bounded. $\alpha = q/\varepsilon$, where q and ε are positive constants denoting the electronic load and the permittivity, respectively. U_T is the thermal voltage. The diffusion $D_s(X)$ depends on the mobility $\mu_s(X)$, i.e., $D_s(X) = U_T\mu_s(X)$, ($s = e$ for the electron and $s = p$ for the hole). $N_D(X)$ and $N_A(X)$ are the donor impurity concentration and acceptor impurity concentration, respectively. $N(X)$, defined by $N(X) = N_D(X) - N_A(X)$, changes rapidly as X approaches nearby the P-N junction. $R_1(e, p, T)$ and $R_2(e, p, T)$ are the recombination rates of the electron, hole and temperature. $\rho(X)$ is the heat transfer coefficient. A nonuniform partition is adopted usually in numerical simulation (He, 1989; Shi, 2002; Yuan, 2009, 2013).

Initial conditions:

$$e(X, 0) = e_0(X),\ p(X, 0) = p_0(X),\ T(X, 0) = T_0(X), \quad X \in \Omega, \tag{5}$$

where $e_0(X)$, $p_0(X)$ and $T_0(X)$ are given positive functions.

In this paper we consider the second type boundary condition (Neumann boundary condition) mainly:

$$\frac{\partial\psi}{\partial\gamma}\Big|_{\partial\Omega} = \frac{\partial e}{\partial\gamma}\Big|_{\partial\Omega} = \frac{\partial p}{\partial\gamma}\Big|_{\partial\Omega} = \frac{\partial T}{\partial\gamma}\Big|_{\partial\Omega} = 0,\ t \in J, \tag{6}$$

where $\partial\Omega$ is the boundary of Ω, and γ is the unit outer normal vector of $\partial\Omega$.

A compatibility condition is added

$$\int_\Omega [p - e + N] dX = 0, \tag{7}$$

and the following condition is given to avoid the ambiguous solution

$$\int_\Omega \psi dX = 0. \tag{8}$$

Numerical simulation of a semiconductor device is important and valuable in manufacturing modern semiconductor (He, 1989; Shi, 2002; Yuan, 2009, 2013). Gummel proposes the sequence iteration to compute the semiconductor problem in 1964 and states a new problem of numerical simulation in semiconductor device (Gummel, 1964). Douglas and Yuan put forward a simple but useful finite difference method and discuss the application and numerical analysis first for the one-dimensional and two-dimensional preliminary problems (constant coefficients and without temperature effect) (Douglas & Yuan, 1987; Yuan, Ding & Yang, 1982), and the research becomes basic theoretical work in numerical simulation of semiconductor device problem. Yuan discusses the characteristic finite element method for variable coefficient problem (Yuan, 1993). Since the diffusion only includes the electric-field strength $-\nabla\psi$, Yuan presents the characteristics-mixed finite element where the concentration is obtained by characteristic finite element and the potential is solved by mixed finite element, and derives optimal-order error estimates in H^1-norm and L^2-norm for a semidiscrete scheme and a fully-discrete method (Yuan, 1991, 19912). There the authors only consider a two-dimensional problem without heat factor, and the index k of mixed finite element space and l of finite element space are restricted by $k \geq 1$ and $l \geq 1$. These features should be improved for actual applications (Jerome, 1994; Yuan, 2009, 2013). Then a characteristic finite element and a characteristic finite difference method are proposed on a uniform partition for a three-dimensional semiconductor device problem of heat conductor (Yuan, 19912, 2000). In this paper the authors put forward a mixed finite element-characteristic mixed finite element for solving a three-dimensional semiconductor device problem, where the potential, concentrations and temperature are computed by a mixed finite element, characteristics-finite element and finite element approximation, respectively. Suppose that $k \geq 0$ and $l \geq 1$. By applying a priori estimates theory and special techniques of differential equations, we obtain optimal-order error estimates in L^2 norm. This composite numerical method shows important suggestions in solving semiconductor problem such as numerical method, software design, actual applications and theoretical and physical study (He, 1989; Jerome, 1994; Shi, 2002; Yuan, 2009, 2013).

2. The Formulation of the Model Problem

To put forward the mixed finite element method-modified method of characteristics (MFEM-MMOC), we reformulate the problem of (1)-(8) as follows

$$\nabla \cdot \mathbf{u} = \alpha\,(p - e + N)\,,\ X \in \Omega, t \in J, \tag{9a}$$

$$\mathbf{u} = -\nabla\psi,\ X \in \Omega, t \in J. \tag{9b}$$

$$\frac{\partial e}{\partial t} - \nabla \cdot (D_e \nabla e) - \mu_e \mathbf{u} \cdot \nabla e - e\mathbf{u} \cdot \nabla\mu_e - \alpha\mu_e(X)e(p - e + N(X)) = -R_1(e, p, T),\ X \in \Omega, t \in J, \tag{10}$$

$$\frac{\partial p}{\partial t} - \nabla \cdot (D_p \nabla p) + \mu_p \mathbf{u} \cdot \nabla p + p\mathbf{u} \cdot \nabla\mu_p + \alpha\mu_p(X)p(p - e + N(X)) = -R_2(e, p, T),\ X \in \Omega, t \in J, \tag{11}$$

$$\rho\frac{\partial T}{\partial t} - \Delta T = \Big\{(D_e(X)\nabla e + \mu_e(X)e\mathbf{u}) - (D_p(X)\nabla p - \mu_p(X)p\mathbf{u})\Big\} \cdot \mathbf{u},\ X \in \Omega, t \in J, \tag{12}$$

$$\mathbf{u} \cdot \gamma = (D_e \nabla e) \cdot \gamma = (D_p \nabla p) \cdot \gamma = \nabla T \cdot \gamma = 0,\ X \in \partial\Omega, t \in J, \tag{13}$$

$$e(X,0) = e_0(X),\ p(X,0) = p_0(X),\ T(X,0) = T_0(X),\ X \in \Omega. \tag{14}$$

Equations (10) and (11) are solved by using MMOC. For convenience to obtain the approximations at the boundary, we suppose that Ω is a cube and the problem of (9)-(14) is Ω-periodic, i.e. all the functions are Ω-periodic. This assumption is reasonable in physical science because mirror reflection is used according to non-permeation condition. Furthermore, the boundary condition (13) can be omitted because it has a small effect on the interior flow of oil reservoirs in common numerical simulations (Ewing, 1984; He, 1989; Shi, 2002; Yuan, 2009, 2013).

Introduce Sobolev space and norms on Ω,

$$\begin{aligned}
&L^2(\Omega) = \{f:\ \int_\Omega |f|^2\, dX < \infty\}, \quad \|f\| = \{\int_\Omega |f|^2 dX\}^{1/2},\\
&L^\infty(\Omega) = \{f:\ \operatorname*{ess\,sup}_\Omega |f| < \infty\}, \quad \|f\|_{L^\infty} = \operatorname*{ess\,sup}_\Omega |f|,\\
&H^m(\Omega) = \{f:\ \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \in L^2(\Omega), |\alpha| \le m\}, \quad \|f\|_m = \Big[\sum_{|\alpha|\le m}\Big\|\frac{\partial^{|\alpha|} f}{\partial x^\alpha}\Big\|^2\Big]^{1/2},\ m \ge 0,\\
&W_\infty^m(\Omega) = \{f:\ \frac{\partial^{|\alpha|} f}{\partial x^\alpha} \in L^\infty(\Omega), |\alpha| \le m\}, \quad \|f\|_{W_\infty^m} = \max_{|\alpha|\le m}\Big\|\frac{\partial^{|\alpha|} f}{\partial x^\alpha}\Big\|_{L^\infty},\ m \ge 0,
\end{aligned}$$

and $H^0(\Omega) = L^2(\Omega)$, $W_\infty^0(\Omega) = L^\infty(\Omega)$. Define inner product in $L^2(\Omega)$

$$(f,g) = \int_\Omega fg dX.$$

The time-dependent space are given. Let $[a,b] \subset J$ and let $\mathbf{X}$ denote a space above. For a function $f(X,t)$ on $\Omega \times [a,b]$, define

$$\begin{aligned}
&H^m(a,b;\mathbf{X}) = \Big\{f:\ \int_a^b \Big\|\frac{\partial^\alpha f}{\partial t^\alpha}\Big\|_{\mathbf{X}}^2 dt < \infty,\ \alpha \le m\Big\},\\
&\|f\|_{H^m(a,b;\mathbf{X})} = \Big\{\sum_{\alpha=0}^m \int_a^b \Big\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\Big\|_{\mathbf{X}}^2 dt\Big\}^{1/2},\ m \ge 0,
\end{aligned}$$

$$\begin{aligned}
&W_\infty^m(a,b;\mathbf{X}) = \Big\{f:\ \operatorname*{ess\,sup}_{[a,b]}\Big\|\frac{\partial^{|\alpha|} f}{\partial t^\alpha}\Big\|_{\mathbf{X}} < \infty, \alpha \le m\Big\},\\
&\|f\|_{W_\infty^m(a,b;\mathbf{X})} = \max_{0\le\alpha\le m}\operatorname*{ess\,sup}_{[a,b]}\Big\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\Big\|_{\mathbf{X}},\ m \ge 0,\\
&L^2(a,b;\mathbf{X}) = H^0(a,b;\mathbf{X}), \quad L^\infty(a,b;\mathbf{X}) = W_\infty^0(a,b;\mathbf{X}).
\end{aligned}$$

For a simple case, $[a,b] = J = [0,\bar{T}]$ and $\mathbf{X} = \Omega$, we omit J and Ω, and replace $L^\infty(0,\bar{T};W_\infty^1(\Omega))$ by $L^\infty(W_\infty^1)$. Then, let

$$\begin{aligned}
&H^m(\mathrm{div}) = \Big\{\mathbf{f}(X) = (f_1,f_2,f_3) : f_1,f_2,f_3,\nabla\cdot\mathbf{f} \in H^m(\Omega)\Big\},\\
&\|\mathbf{f}\|_{H^m(\mathrm{div})} = \Big(\sum_{i=1}^3 \|f_i\|_{H^m}^2 + \|\nabla\cdot\mathbf{f}\|_m^2\Big)^{1/2},\ m \ge 0,\\
&H(\mathrm{div}) = H^0(\mathrm{div}).
\end{aligned}$$

Suppose that the problem of (9)-(14) is regular,

$$(R) \quad \left\{\begin{array}{l}
\psi \in L^\infty(H^{k+1},\\
\mathbf{u} \in L^\infty(H^{k+1}(\mathrm{div})) \bigcap L^\infty(W_\infty^1) \bigcap W_\infty^1(L^\infty) \bigcap H^2(L^2),\\
e,p,T \in L^\infty(H^{l+1}) \bigcap H^1(H^{l+1}) \bigcap L^\infty(W_\infty^1) \bigcap H^2(L^2).
\end{array}\right. \tag{15}$$

Here $l \ge 1$ and $k \ge 0$ are integers, and they denote the degrees of polynomials approximating e,p,T and ψ.

The coefficients of (9)-(14) are positive definite,

$$(C) \quad \left\{\begin{array}{l}
0 < D_* \le D_s(X) \le D^*, \quad 0 < \mu_* \le \mu_s(X) \le \mu^*, s = e,p,\\
0 < \rho_* \le \rho(X) \le \rho^*, \quad |\nabla\mu_s| \le K^*, s = e,p,
\end{array}\right. \tag{16}$$

where $D_*, D^*, \mu_*, \mu^*, \rho_*, \rho^*$ and K^* are positive constants. Suppose that $R_1(e,p,T)$ and $R_2(e,p,T)$ are Lipschitz continuous on a ε_0-neighborhood of X.

3. The Procedures of MFEM-MMOC

Numerical scheme of (9)-(14) is constructed in this section. A mixed finite element method (MFEM), a modified method of characteristics (MMOC) and a finite element method (FEM) are used to solve the potential, the electron and hole concentrations, and the temperature, respectively.

3.1 The MFEM for Potential

Eq. (1) is reformulated by (9a) and (9b). Test both sides of (9b) by $\mathbf{v} \in H(\mathrm{div})$, obtain an inner product equation on Ω and apply the divergence theorem for the term dependent on $\nabla\psi$. Eq. (9a) is treated similarly. Then, we have a saddle-point problem of (9): to find $(\mathbf{u}(X,t), \psi(X,t)) \in H(\mathrm{div}) \times L^2(\Omega)$ such that

$$\int_\Omega \mathbf{u}\cdot\mathbf{v}dX - \int_\Omega \psi\nabla\cdot\mathbf{v}dX = 0, \quad \mathbf{v}\in H(\mathrm{div}), \tag{17a}$$

$$\int_\Omega w\nabla\cdot\mathbf{u}dX = \int_\Omega \alpha(p-e+N(X))wdX, \quad w\in L^2(\Omega). \tag{17b}$$

Introduce the time-dependent partition and finite element space. Let $\Omega = \bigcup\Omega_e$ be a quasiuniform partition with diameter h_p. Let $V^k \subset H(\mathrm{div})$ and $S_p^k \subset L^2(\Omega)$ denote the k-order mixed finite element spaces, $k \geq 0$. The time partition is defined by $0 = t_0^p < t_1^p < \cdots < t_m^p < \cdots < t_{M-1}^p < t_M^p = \bar{T}$, and $\Delta t_m^p = t_m^p - t_{m-1}^p$, $\Delta t_p = \max\limits_{1\leq m\leq M} \Delta t_m^p$.

Given $e_h(X,t_m^p)$, $p_h(X,t_m^p)$ at t_m^p, MFEM is used to compute $\mathbf{u}_h(X,t_m^p) \in \mathbf{V}^k$ and $\psi_h(X,t_m^p) \in S_\psi^k$,

$$\int_\Omega \mathbf{u}_h(X,t_m^p)\cdot\mathbf{v}_h(X)dX - \int_\Omega \psi_h(X,t_m^p)\nabla\cdot\mathbf{v}_h(X)dX = 0, \quad \mathbf{v}_h(X)\in\mathbf{V}^k, \tag{18a}$$

$$\int_\Omega w_h(X)\nabla\cdot\mathbf{u}_h(X,t_m^p)dX = \int_\Omega \alpha_h(p_h(X,t_m^p) - e_h(X,t_m^p) + N(X))w_h(X)dX, \quad w_h(X)\in S_\psi^k. \tag{18b}$$

3.2 The MMOC for Concentrations

Generally, the strength changes slower than the concentrations and the computational cost in space and time is more expensive when the MFEM (18) used at each time level. Thus, a larger time step is adopted for the potential equation. For convenience, the partition for concentrations is obtained by refining the meshes of the potential, $0 = t_0^c < t_1^c < \cdots < t_n^c < \cdots < t_{N-1}^c < t_{N_1}^c = t_1^p < t_{N_1+1}^c < \cdots < t_{N_2}^c = t_2^p < \cdots < t_{N_M-1}^c < t_{N_M}^c = t_M^p = \bar{T}$. Let $\Delta t_n^c = t_n^c - t_{n-1}^c$ and $\Delta t_c = \max\limits_{1\leq n\leq N_M} \Delta t_n^c$. During the computation of MMOC, we should define an extrapolation of $\mathbf{u}_h(X,t_{m-2}^p)$ and $\mathbf{u}_h(X,t_{m-1}^p)$, denoted by $E\mathbf{u}_h(X,t_n^c)$, to approximate the value at t_n^c, $t_{m-1}^p < t_n^c < t_m^p$,

$$E\mathbf{u}_h(X,t_n^c) = \begin{cases} (1+\frac{t_n^c - t_{m-1}^p}{\Delta t_{m-1}^p})\mathbf{u}_h(X,t_{m-1}^p) - \frac{t_n^c - t_{m-1}^p}{\Delta t_{m-1}^p}\mathbf{u}_h(X,t_{m-2}^p), & N_{m-1}\leq n\leq N_m, 2\leq m\leq M,\\ \mathbf{u}_h(X,0), & 1\leq n\leq N_1, m=1. \end{cases} \tag{19}$$

The MMOC is defined now for (10) and (11). Let denote a unit vector τ_e of $(-\mu_e E\mathbf{u}, 1)$ in the composite space $\Omega\times[0,\bar{T}]$, and let $\phi_e(X) = \left(|\mu_e E\mathbf{u}(X)|^2 + 1\right)^{1/2}$. Then,

$$\phi_e\frac{\partial e(X,t_n^c)}{\partial\tau_e} = \frac{\partial e}{\partial t}(X,t_n^c) - \mu_e E\mathbf{u}(X,t_n^c)\cdot\nabla e(X,t_n^c). \tag{20}$$

It is approximated by using the characteristic finite difference,

$$\phi_e\frac{\partial e}{\partial\tau_e}(X,t_n^c) \approx \phi_e\frac{e(X,t_n^c) - e(\check{X}_e^{n-1},t_{n-1}^c)}{\Delta t_n^c\left(|\mu_e E\mathbf{u}(X)|^2+1\right)^{1/2}} = \frac{e(X,t_n^c) - e(\check{X}_e^{n-1},t_{n-1}^c)}{\Delta t_n^c}, \tag{21}$$

where $\check{X}_e^{n-1} = X + \mu_e E\mathbf{u}(X,t_n^c)\Delta t_n^c$. Furthermore,

$$\phi_e\frac{\partial e}{\partial\tau_e}(X,t_n^c) - \frac{e(X,t_n^c) - e(\check{X}_e^{n-1},t_{n-1}^c)}{\Delta t_n^c} = \frac{1}{\Delta t_n^c}\int_{(\check{X}_e^{n-1},t_{n-1}^c)}^{(X,t_n^c)} \left[(X-\check{X}_e^{n-1})^2 + (\tau_e - t_{n-1}^c)^2\right]^{1/2}\frac{\partial^2 e}{\partial\tau_e^2}d\tau_e. \tag{22}$$

The hole concentration equation (11) is discussed similarly. τ_p is a unit vector of $(\mu_p E\mathbf{u}, 1)$. Let $\phi_p(X) = \left(\left|\mu_p E\mathbf{u}(X)\right|^2 + 1\right)^{1/2}$, then we have

$$\phi_p\frac{\partial p(X,t_n^c)}{\partial\tau_p} = \frac{\partial p}{\partial t}(X,t_n^c) + \mu_p E\mathbf{u}(X,t_n^c)\cdot\nabla p(X,t_n^c). \tag{23}$$

The characteristic derivative is treated by

$$\phi_p \frac{\partial p}{\partial \tau_p}(X, t_n^c) \approx \phi_p \frac{p(X, t_n^c) - p(\check{X}_p^{n-1}, t_{n-1}^c)}{\Delta t_n^c(\left|1 + \mu_p E\mathbf{u}(X)\right|^2)^{1/2}} = \frac{p(X, t_n^c) - p(\check{X}_p^{n-1}, t_{n-1}^c)}{\Delta t_n^c}, \tag{24}$$

where $\check{X}_p^{n-1} = X - \mu_p E\mathbf{u}(X, t_n^c)\Delta t_n^c$. Furthermore,

$$\phi_p \frac{\partial p}{\partial \tau_p}(X, t_n^c) - \frac{p(X, t_n^c) - p(\check{X}_p^{n-1}, t_{n-1}^c)}{\Delta t_n^c} = \frac{1}{\Delta t_n^c} \int_{(\check{X}_p^{n-1}, t_{n-1}^c)}^{(X, t_n^c)} \left[(X - \check{X}_p^{n-1})^2 + (\tau_p - t_{n-1}^c)^2\right]^{1/2} \frac{\partial^2 p}{\partial \tau_p^2} d\tau_p. \tag{25}$$

During the computations, the space step h_p for the potential is larger than that for the concentrations and temperature, i.e., $h_p > h_c$. $S_c^l \subset W_\infty^1(\Omega)$ denotes a finite element space for the concentrations and temperature consisting of all the piecewise polynomial functions of degree at most l, $l \geq 1$. $e_h(X, 0), p_h(X, 0)$ and $T_h(X, 0)$ are approximations of $e_0(X), p_0(X)$ and $T_0(X)$, where Ritz projection and interpolations are used generally. Then MFEM-MMOC for solving the problem of (9)-(14) follows.

(1) Initial approximations are given by

$$e_h(X, 0), p_h(X, 0), T_h(X, 0) \quad X \in \Omega. \tag{26}$$

(2) Given $e_h(X, t_{m-1}^p)$, $p_h(X, t_{m-1}^p)$ and $T_h(X, t_{m-1}^p)$, numerical solutions at t_n^c for $n = N_{m-1} + 1, N_{m-1} + 2, \cdots, N_m$, $e_h(X, t_n^c) \times p_h(X, t_n^c) \times T_h(X, t_n^c) \in S_c^l \times S_c^l \times S_c^l$ are computed by

$$\begin{aligned}
&\int_\Omega \frac{e_h(X, t_n^c) - \hat{e}_h(X, t_{n-1}^c)}{\Delta t_n^c} Z_h dX + \int_\Omega D_e(X)\nabla e_h(X, t_n^c) \cdot \nabla Z_h dX - \int_\Omega e_h(X, t_n^c) E\mathbf{u}_h(X, t_n^c) \cdot \nabla \mu_e Z_h dX \\
&- \alpha \int_\Omega \mu_e e_h(X, t_n^c)(p_h(X, t_{n-1}^c) - e_h(X, t_{n-1}^c) + N(X)) Z_h dX \\
&= - \int_\Omega R_1(e_h(X, t_{n-1}^c), p_h(X, t_{n-1}^c), T_h(X, t_{n-1}^c)) Z_h dX, \ \forall\, Z_h \in S_c^l,
\end{aligned} \tag{27a}$$

where $\hat{e}_h(X, t_{n-1}^c) = e_h(\hat{X}_e, t_{n-1}^c)$, $\hat{X}_e = X + \mu_e E\mathbf{u}_h(X, t_n^c)\Delta t_n^c$.

$$\begin{aligned}
&\int_\Omega \frac{p_h(X, t_n^c) - \hat{p}_h(X, t_{n-1}^c)}{\Delta t_n^c} Z_h dX + \int_\Omega D_p(X)\nabla p_h(X, t_n^c) \cdot \nabla Z_h dX - \int_\Omega p_h(X, t_n^c) E\mathbf{u}_h(X, t_n^c) \cdot \nabla \mu_p Z_h dX \\
&+ \alpha \int_\Omega \mu_p p_h(X, t_n^c)(p_h(X, t_{n-1}^c) - e_h(X, t_{n-1}^c) + N(X)) Z_h dX \\
&= - \int_\Omega R_2(e_h(X, t_{n-1}^c), p_h(X, t_{n-1}^c), T_h(X, t_{n-1}^c)) Z_h dX, \ \forall\, Z_h \in S_c^l,
\end{aligned} \tag{27b}$$

where $\hat{p}_h(X, t_{n-1}^c) = p_h(\hat{X}_p, t_{n-1}^c)$, $\hat{X}_p = X - \mu_p E\mathbf{u}_h(X, t_n^c)\Delta t_n^c$,

$$\begin{aligned}
&\int_\Omega \rho(X) \frac{T_h(X, t_n^c) - T_h(X, t_{n-1}^c)}{\Delta t_n^c} Z_h dX + \int_\Omega \nabla T_h(X, t_n^c) \cdot \nabla Z_h dX \\
&= \int_\Omega \{(D_e \nabla e_h(X, t_{n-1}^c) + \mu_e e_h(X, t_{n-1}^c) E\mathbf{u}_h(X, t_n^c)) \\
&\quad - (D_p \nabla p_h(X, t_{n-1}^c) - \mu_p p_h(X, t_{n-1}^c) E\mathbf{u}_h(X, t_n^c))\} \cdot E\mathbf{u}_h(X, t_n^c) Z_h dX, \ \forall\, Z_h \in S_c^l.
\end{aligned} \tag{27c}$$

(3) When $e_h(X, t_m^p)$ and $p_h(X, t_m^p)$ are computed, then the potential and strength at t_m^p, $\mathbf{u}_h(X, t_m^p) \in \mathbf{V}^k$ and $\psi_h(X, t_m^p) \in S_\psi^k$ are obtained by

$$\int_\Omega \mathbf{u}_h(X, t_m^p) v_h(X) dX - \int_\Omega \psi_h(X, t_m^p) \nabla \cdot \mathbf{v}_h dX = 0, \ \forall\, \mathbf{v}_h \in \mathbf{V}^k, \tag{28a}$$

$$\int_\Omega w_h(X) \nabla \cdot \mathbf{u}_h(X, t_m^p) dX = \alpha \int_\Omega (p_h(X, t_m^p) - e_h(X, t_m^p) + N(X)) w_h(X) dX, \ \forall\, w_h \in S_\psi^k. \tag{28b}$$

MFEM-MMOC runs as follows. First (26) is determined by using the Ritz projection (see the following section) or interpolations. Then by using (27), $e_h(X, t_n^c), p_h(X, t_n^c), T_h(X, t_n^c)$ are computed at $n = N_{m-1} + 1, N_{m-1} + 2, \cdots, N_m$. (28)

is used to obtain $\mathbf{u}_h(X, t_m^p), \psi_h(X, t_m^p)$ at t_m^p. The procedures of (27) and (28) are used repeatedly and all the numerical solutions are obtained. According to (C), numerical solutions exist and are unique.

4. Preliminary Estimates

Suppose that the following approximation property and inverse property hold

$$(\mathrm{A_c}) \quad \inf_{Z_h \in S_c^l} \left\{ \|Z - Z_h\|_{L^2} + h_c \|Z - Z_h\|_{H^1} \right\} \le A_1 h_c^m \|Z\|_{H^m}, \ \forall\, Z \in H^m(\Omega), 2 \le m \le l+1, \tag{29}$$

$$(\mathrm{I_c}) \quad \begin{array}{l} \|Z_h\|_{H^1} \le K_1 h_c^{-1} \|Z_h\|_{L^2}, \quad \|Z_h\|_{L^\infty} \le K_1 (1 + \ln \frac{1}{h})^{1-\frac{l}{3}} h_c^{-\frac{1}{2}} \|Z_h\|_{H^1}, \\ \|Z_h\|_{W_\infty^m} \le K_1 h_c^{-3/2} \|Z_h\|_{H^m}, \ \forall\, Z_h \in S_c^l, \end{array} \tag{30}$$

where A_1 and K_1 are positive constants independent of h_c.

Similarly, $\{\mathbf{V}^k, S_\psi^k\}$ has the following properties

$$(\mathrm{A_p}) \quad \begin{array}{l} \inf_{w_h \in S_\psi^k} \|w - w_h\|_{L^2} \le A_2 h_p^m \|w\|_{H^m}, \quad \forall\, w \in H^m, \\ \inf_{\mathbf{v}_h \in \mathbf{V}^k} \|\mathbf{v} - \mathbf{v}_h\|_{H(\mathrm{div})} \le A_2 h_p^m \|\mathbf{v}\|_{H^m(\mathrm{div})}, \quad \forall\, \mathbf{v} \in H^m(\mathrm{div}), \\ \inf_{w_h \in S_\psi^k} \|w - w_h\|_{L^2} \le A_2 h_p^m \|w\|_{H^m}, \quad \forall\, w \in H^m, \ 1 \le m \le k+1, \end{array} \tag{31}$$

$$(\mathrm{I_p}) \quad \begin{array}{l} \|\mathbf{v}\|_{L^\infty} \le K_2 h_p^{-3/2} \|\mathbf{v}\|_{L^2}, \quad \forall\, \mathbf{v} \in \mathbf{V}^k, \\ \|\mathbf{v}\|_{W_\infty^1(\mathcal{J})} \le K_2 h_p^{-1} \|\mathbf{v}\|_{L^\infty(\mathcal{J})}, \ \mathcal{J} \text{ is a partition element}, \end{array} \tag{32}$$

where A_2 and K_2 are positive constants independent of h_p.

The Ritz projection of $e(X,t)$, $\Pi e(X,t) \in S_c^l, t \in (0, \bar{T}]$, is defined by

$$\begin{aligned} &\int_\Omega \nabla\chi(X) \cdot D_e(X) \nabla \Pi e(X,t) dX + \int_\Omega \chi(X) \Pi e(X,t) dX \\ &= \int_\Omega \nabla\chi(X) \cdot D_e(X) \nabla e(X,t) dX + \int_\Omega \chi(X) e(X,t) dX \\ &= -\int_\Omega \chi(X) \frac{\partial e}{\partial t}(X,t) dX + \int_\Omega \chi(X) \mu_e \mathbf{u}(X,t) \cdot \nabla e(X,t) dX \\ &- \int_\Omega \chi(X) e(X,t) \mathbf{u}(X,t) \cdot \nabla \mu_e dX + \int_\Omega \chi(X) [\alpha \mu_e e(X,t)(p(X,t) - e(X,t) + N(X))] dX \\ &+ \int_\Omega \chi(X) e(X,t) dX - \int_\Omega \chi(X) R_1(e(X,t), p(X,t), T(X,t)) dX, \ \forall\, \chi(X) \in S_c^l. \end{aligned} \tag{33}$$

According to the discussions (Ewing, 1984; Russell, 1980; Wheeler, 1973), we have

$$\begin{aligned} &\|e - \Pi e\|_{L^\infty(L^2)} + h_c \|e - \Pi e\|_{L^\infty(H^1)} \le A_1 h_c^m \|e\|_{L^\infty(H^m)}, \\ &\left\| \frac{\partial}{\partial t}(e - \Pi e) \right\|_{L^\infty(L^2)} \le A_1 h_c^m \|e\|_{H^1(H^m)}, \ 2 \le m \le l+1, \\ &\|\Pi e\|_{L^\infty(W_\infty^1)} \le A_1, \end{aligned} \tag{34}$$

where A_1 is independent of e and h_c.

The Ritz projection of $p(X,t)$, $\Pi p(X,t) \in S_c^l, t \in (0, \bar{T}]$, is defined by

$$\begin{aligned} &\int_\Omega \nabla\chi(X) \cdot D_p(X) \nabla \Pi p(X,t) dX + \int_\Omega \chi(X) \Pi p(X,t) dX \\ &= \int_\Omega \nabla\chi(X) \cdot D_p(X) \nabla p(X,t) dX + \int_\Omega \chi(X) p(X,t) dX \\ &= -\int_\Omega \chi(X) \frac{\partial p}{\partial t}(X,t) dX - \int_\Omega \chi(X) \mu_p \mathbf{u}(X,t) \cdot \nabla p(X,t) dX \\ &- \int_\Omega \chi(X) p(X,t) \mathbf{u}(X,t) \cdot \nabla \mu_p dX - \int_\Omega \chi(X) \alpha \mu_p p(X,t)(p(X,t) - e(X,t) + N(X)) dX \\ &+ \int_\Omega \chi(X) p(X,t) dX - \int_\Omega \chi(X) R_2(e(X,t), p(X,t), T(X,t)) dX, \ \forall\, \chi(X) \in S_c^l, \end{aligned} \tag{35}$$

and it holds

$$\begin{aligned}
&\|p - \Pi p\|_{L^\infty(L^2)} + h_c \|p - \Pi p\|_{L^\infty(H^1)} \le A_1 h_c^m \|p\|_{L^\infty(H^m)}, \\
&\left\|\frac{\partial}{\partial t}(p - \Pi p)\right\|_{L^\infty(L^2)} \le A_1 h_c^m \|p\|_{H^1(H^m)},\ 2 \le m \le l+1, \\
&\|\Pi p\|_{L^\infty(W^1_\infty)} \le A_1,
\end{aligned} \tag{36}$$

where A_1 is independent of p and h_c.

The Ritz projection of $T(X,t)$, $\Pi T(X,t) \in S^l_c, t \in (0, \bar{T}]$, is defined by

$$\begin{aligned}
&\int_\Omega \nabla\chi(X)\cdot\nabla\Pi T(X,t)dX + \int_\Omega \chi(X)\Pi T(X,t)dX \\
&= \int_\Omega \nabla\chi(X)\cdot\nabla T(X,t)dX + \int_\Omega \chi(X)T(X,t)dX \\
&= -\int_\Omega \chi(X)\rho\frac{\partial T}{\partial t}(X,t)dX + \int_\Omega \chi(X)T(X,t)dX - \int_\Omega \chi(X)\{(D_p(X)\nabla p(X,t) - \mu_p p(X,t)\mathbf{u}(X,t)) \\
&\quad - (D_e(X)\nabla e(X,t) - \mu_e e(X,t)\mathbf{u}(X,t))\}\mathbf{u}(X,t)dX,\ \forall\, \chi(X) \in S^l_c.
\end{aligned} \tag{37}$$

Similarly,

$$\begin{aligned}
&\|T - \Pi T\|_{L^\infty(L^2)} + h_c \|T - \Pi T\|_{L^\infty(H^1)} \le A_1 h_c^m \|T\|_{L^\infty(H^m)}, \\
&\left\|\frac{\partial}{\partial t}(T - \Pi T)\right\|_{L^\infty(L^2)} \le A_1 h_c^m \|T\|_{H^1(H^m)},\ 2 \le m \le l+1, \\
&\|\Pi T\|_{L^\infty(W^1_\infty)} \le A_1,
\end{aligned} \tag{38}$$

where A_1 is independent of T and h_c.

The projection of $(\mathbf{u}, \psi) \in H(\mathrm{div}) \times L^2$, $(\Pi\mathbf{u}, \Pi\psi) \in \mathbf{V}^k \times S^k_\psi$, is defined by

$$\int_\Omega (\Pi\mathbf{u}(X,t) - \mathbf{u}(X,t))\cdot\mathbf{v}(X)dX - \int_\Omega (\Pi\psi(X,t) - \psi(X,t))\nabla\cdot\mathbf{v}(X)dX = 0,\ \forall\, \mathbf{v} \in \mathbf{V}^k, \tag{39a}$$

$$\int_\Omega \nabla\cdot(\Pi\mathbf{u}(X,t) - \mathbf{u}(X,t))w(X)dX = 0,\ \forall\, w(X) \in S^k_\psi. \tag{39b}$$

Then it follows from the discussion of Raviart-Thomas (Brezzi, 1974; Douglas, 1983)

$$\|\Pi\mathbf{u} - \mathbf{u}\|_{L^\infty(H(\mathrm{div}))} + \|\Pi\psi - \psi\|_{L^\infty(L^2)} \le A_2(\, \|\mathbf{u}\|_{L^\infty(H(\mathrm{div}))} + \|\mathbf{u}\|_{L^\infty(H^{k+1})}\, h_p^{k+1}, \tag{40a}$$

$$\|\Pi\mathbf{u}\|_{L\infty(L^\infty)} \le A_2 h_p^{-1/2}, \tag{40b}$$

where A_2 is independent of $h_p, \mathbf{u}, \psi$ and e, p.

Define an extrapolation of $\mathbf{u}$,

$$E\mathbf{u}(X, t^c_n) = \begin{cases} (1 + \frac{t^c_n - t^p_{m-1}}{\Delta t^p_{m-1}})\mathbf{u}(X, t^p_{m-1}) - \frac{t^c_n - t^p_{m-1}}{\Delta t^p_{m-1}}\mathbf{u}(X, t^p_{m-2}), & N_{m-1} \le n \le N_m, 2 \le m \le M, \\ \mathbf{u}(X, 0), & 1 \le n \le N_1, m = 1. \end{cases} \tag{41}$$

Furthermore,

$$\|E\mathbf{u}(X,t) - \mathbf{u}(X,t)\|_{L^2} \le \begin{cases} A_3(\Delta t_p)^{3/2}\|u\|_{H^2(t^p_{m-2}, t^p_m; L^2)}, & t \in [t^p_{m-1}, t^p_m], m \ge 2, \\ A_3\Delta t^1_p \|u\|_{W^1_\infty(t^p_0, t^p_1; L^2)}, & m = 1, \end{cases} \tag{42}$$

where A_3 is a positive constant.

5. Convergence Analysis

For simplicity, Δt_c and Δt_p are supposed to be independent of the time. Then, MFEM-MMOC is reformulated as follows to compute numerical solutions $\{e_h, p_h, T_n\}$:$\{t^1, t^2, \cdots, t^N\} \to S_c^l \times S_c^l \times S_c^l$, $\{\mathbf{u}_h, \psi_h\} : \{t_1, t_2, \cdots, t_M\} \to \mathbf{V}^k \times S_\psi^k$:

$$e_h^0 = \Pi e^0,\ p_h^0 = \Pi p^0,\ T_h^0 = \Pi T^0,\ X \in \Omega. \tag{43}$$

$$\begin{aligned}
&\Big(\frac{e_h^n - \hat{e}_h^{n-1}}{\Delta t^c}, Z_h\Big) + (D_e \nabla e_h^n, \nabla Z_h) - (e_h^n E \mathbf{u}_h^n \cdot \nabla \mu_e, Z_h) - \alpha(\mu_e e_h^n (p_h^{n-1} - e_h^{n-1} + N(X)), Z_h) \\
&= -(R_1(e_h^{n-1}, p_h^{n-1}, T_h^{n-1}), Z_h),\ \forall\, Z_h \in S_c^l, && (44a)\\
&\Big(\frac{p_h^n - \hat{p}_h^{n-1}}{\Delta t_c}, Z_h\Big) + (D_p \nabla p_h^n, \nabla Z_h) - (p_h^n E \mathbf{u}_h^n \cdot \nabla \mu_p, Z_h) + \alpha(\mu_p p_h^n (p_h^{n-1} - e_h^{n-1} + N(X)), Z_h) \\
&= -(R_2(e_h^{n-1}, p_h^{n-1}, T_h^{n-1}), Z_h),\ \forall\, Z_h \in S_c^l, && (44b)\\
&\Big(\rho \frac{T_h^n - T_h^{n-1}}{\Delta t_c}, Z_h\Big) + (\nabla T_h^n, \nabla Z_h) \\
&= \Big(\{(D_e \nabla e_h^{n-1} + \mu_e e_h^{n-1} E \mathbf{u}_h^n) - (D_p \nabla p_h^{n-1} - \mu_p p_h^{n-1} E \mathbf{u}_h^n)\} \cdot E \mathbf{u}_h^n, Z_h\Big),\ \forall\, Z_h \in S_c^l, && (44c)
\end{aligned}$$

where $\hat{e}_h^{n-1} = e_h^{n-1}(\hat{X}_e)$, $\hat{X}_e = X + \mu_e E \mathbf{u}_h^n \Delta t_c$, $\hat{p}_h^{n-1} = p_h^{n-1}(\hat{X}_p)$, $\hat{X}_p = X - \mu_p E \mathbf{u}_h^n \Delta t_c$.

$$(\mathbf{u}_{h,m}, v_h) - (\psi_{h,m}, \nabla \cdot \mathbf{v}_h) = 0,\ \forall\, \mathbf{v}_h \in \mathbf{V}^k, \tag{45a}$$

$$(\nabla \cdot \mathbf{u}_{h,m}, w_h) = \alpha(p_{h,m} - e_{h,m} + N(X), w_h),\ \forall\, w_h \in S_\psi^k. \tag{45b}$$

Given e_h^0, p_h^0, T_h^0t, by using (45), $\mathbf{u}_{h,0}$ and $\psi_{h,0}$ are obtained. Then from (44) we get $\{e_h^1, p_h^1, T_h^1\}$, $\{e_h^2, p_h^2, T_h^2\}, \cdots, \{e_h^{N_1}, p_h^{N_1}, T_h^{N_1}\}$. Note that $t^{N_1} = t_1$, we compute $\{\mathbf{u}_{h,1}, \psi_{h,1}\}$ by (45). All the numerical solutions are obtained after repeated computations.

In the following discussions, the symbols K and ε denote a generic positive constant and a generic small positive number, respectively. They can take different values at different places.

The optimal error estimates for $k \geq 0$ and $l \geq 1$ follow.

Theorem 1 *Suppose that $\psi, \mathbf{u}, e, p, T$ are exact solutions of (1)-(8) and satisfy $\psi \in L^\infty(H^{k+1})$, $\mathbf{u} \in L^\infty(H^{k+1}(\mathrm{div})) \bigcap W_\infty^1(L^\infty) \bigcap H^2(L^2)$, $e, p, T \in L^\infty(H^{l+1}) \bigcap H^1(H^{l+1}) \bigcap L^\infty(W_\infty^1) \bigcap H^2(L^2)$. Let $\psi_h, \mathbf{u}_h, e_h, p_h, T_h$ be numerical solutions of (43)-(45). Suppose that $k \geq 0$, $l \geq 1$, and the following partition constrict holds*

$$\Delta t_c = o(h_p),\ h_c^{l+1} = O(h_p),\ (\Delta t_p^1)^{3/2} = O(h_p),\ (\Delta t_p)^2 = O(h_p). \tag{46}$$

Then,

$$\begin{aligned}
&\|\mathbf{u}_h - \mathbf{u}\|_{L^\infty(H(\mathrm{div}))} + \|\psi_h - \psi\|_{L^\infty(L^2)} + \sum_{s=e,p,T} \Big\{ \|s_h - s\|_{L^\infty(L^2)} + \|s_h - s\|_{L^2(H^1)} \Big\} \\
&\leq K^* \Delta t_c \Big\{ \sum_{s=e,p,T} \Big\| \frac{\partial^2 s}{\partial \tau_s^2} \Big\|_{L^2(L^2)} + \Big\| \frac{\partial^2 T}{\partial t^2} \Big\|_{L^2(L^2)} \Big\} + K^* \Big\{ (\Delta t_{p,1})^{3/2} + (\Delta t_p)^2 \Big\} \|\mathbf{u}\|_{H^1(L^2)} \\
&\quad + K^* h_c^{l+1} \sum_{s=e,p,T} \Big\{ \|s\|_{L^\infty(H^{l+1})} + \|s\|_{H^1(H^{l+1})} \Big\} + K^* h_p^{k+1} \Big\{ \|u\|_{L^\infty(H^{k+1}(\mathrm{div}))} + \|\psi\|_{L^\infty(H^{k+1})} \Big\},
\end{aligned} \tag{47}$$

where K^* is a positive constant independent of $h_c, h_p, \Delta t_p^1$ and Δt_p.

Proof. The electric potential equation is considered first. Subtracting (39) at $t = t_m$ from (28), we get

$$(\mathbf{u}_{h,m} - \Pi \mathbf{u}_m, v_h) - (\psi_{h,m} - \Pi \psi_m, \nabla \cdot \mathbf{v}_h) = 0,\ \forall\, \mathbf{v}_h \in \mathbf{V}^k, \tag{48a}$$

$$(\nabla \cdot (\mathbf{u}_{h,m} - \mathbf{u}_m), w_h) = \alpha(p_{h,m} - p_m - e_{h,m} + e_m, w_h),\ \forall\, w_h \in S_\psi^k. \tag{48b}$$

From the Brezzi's discussion of saddle-point problem (Brezzi, 1974; Douglas, 1983) and eq. (40), we have

$$\big\|\mathbf{u}_{h,m} - \Pi \mathbf{u}_m\big\|_{H(\mathrm{div})} + \big\|\psi_{h,m} - \Pi \psi_m\big\|_{L^2} \leq K \sum_{s=e,p} \big\|s_{h,m} - s_m\big\|, \tag{49}$$

then we get

$$\begin{aligned}
\|E(\mathbf{u}^n - \Pi\mathbf{u}^n)\| &\le K\Big\{ \|\mathbf{u}_{m-1} - \Pi\mathbf{u}_{m-1}\| + \|\mathbf{u}_{m-2} - \Pi\mathbf{u}_{m-2}\| \Big\} \\
&\le K\Big\{ \|\psi\|_{L^\infty(H^{k+1})}, \|u\|_{L^\infty(H^{k+q}(\mathrm{div}))} \Big\} h_p^{k+1}, \qquad (50a) \\
\left\|E(\mathbf{u}_h^n - \Pi\mathbf{u}^n)\right\| &\le K\Big\{ \sum_{s=e,p} \|s\|_{L^\infty(H^{l+1})} \Big\} h_c^{l+1} + \sum_{s=e,p} \Big[\|(s_h - \Pi s_h)_{m-1}\| + \|(s_h - \Pi s_h)_{m-2}\| \Big]. \qquad (50b)
\end{aligned}$$

From (40) and (49), it is necessary to show optimal error estimates of $\sum_{s=e,p} \|s_h - s\|_{L^\infty(L^2)}$ to complete the proof of (47).

Let $\xi_e^n = e_h^n - \Pi e^n$, $\eta_e^n = \Pi e^n - e^n$, $\xi_p^n = p_h^n - \Pi p^n$, $\eta_p^n = \Pi p^n - p^n$, $\xi_T^n = T_h^n - \Pi T^n$ and $\eta_T^n = \Pi T^n - T^n$. Subtracting (33) ($t = t^n$) from (44a), we obtain error equation of electron concentration

$$\begin{aligned}
&\Big(\frac{\xi_e^n - \xi_e^{n-1}}{\Delta t_c}, Z_h\Big) + (D_e\nabla\xi_e^n, \nabla Z_h) - (\mu_e[\mathbf{u} - E\mathbf{u}^n]\cdot\nabla e^n, Z_h) - ([e_h^n E\mathbf{u}_h^n - e^n\mathbf{u}^n]\cdot\nabla\mu_e, Z_h) \\
&- \alpha(\mu_e[e_h^n(p_h^{n-1} - e_h^{n-1} + N(X)) - e^n(p^n - e^n + N(X))], Z_h) \\
&= \Big([\frac{\partial e^n}{\partial t} - \mu_e E\mathbf{u}^n\cdot\nabla e^n] - \frac{e^n - \check{e}^n}{\Delta t_c}, Z_h\Big) - \Big(\frac{\eta_e^n - \eta_e^{n-1}}{\Delta t_c}, Z_h\Big) + (\eta_e^n, Z_h) \qquad (51) \\
&- (R_1(e_h^{n-1}, p_h^{n-1}, T_h^{n-1}) - R_1(e_h^n, p_h^n, T_h^n), Z_h) + \Big(\frac{\hat{e}^{n-1} - \check{e}^{n-1}}{\Delta t_c}, Z_h\Big) + \Big(\frac{\hat{\eta}_e^{n-1} - \check{\eta}_e^{n-1}}{\Delta t_c}, Z_h\Big) \\
&+ \Big(\frac{\xi_e^{n-1} - \check{\xi}_e^{n-1}}{\Delta t_c}, Z_h\Big) + \Big(\frac{\check{\eta}_e^{n-1} - \eta_e^{n-1}}{\Delta t_c}, Z_h\Big) + \Big(\frac{\check{\xi}_e^{n-1} - \xi_e^{n-1}}{\Delta t_c}, Z_h\Big),\ \forall\, Z_h \in S_c^l,\ n \ge 1.
\end{aligned}$$

Take $Z_h = \xi_e^n$ to get an L^2-norm result. The first term on the left-hand side is estimated by

$$\Big(\frac{\xi_e^n - \xi_e^{n-1}}{\Delta t_c}, \xi_e^n\Big) \ge \frac{1}{2\Delta t_c}\Big\{ \left\|\xi_e^n\right\|^2 - \left\|\xi_e^{n-1}\right\|^2 \Big\}. \qquad (52)$$

Then, we have

$$\begin{aligned}
&\frac{1}{2\Delta t_c}\{ \left\|\xi_e^n\right\|^2 - \left\|\xi_e^{n-1}\right\|^2 \} + (D_e\nabla\xi_e^n, \nabla\xi_e^n) \\
&\le \Big([\frac{\partial e^n}{\partial t} - \mu_e E\mathbf{u}^n\cdot\nabla e^n] - \frac{e^n - \check{e}^{n-1}}{\Delta t_c}, \xi_e^n\Big) + (\mu_e[\mathbf{u} - E\mathbf{u}^n]\cdot\nabla e^n, \xi_e^n) + ([e_h^n E\mathbf{u}_h^n - e^n\mathbf{u}^n]\cdot\nabla\mu_e, \xi_e^n) \\
&+ \alpha(\mu_e[e_h^n(p_h^{n-1} - e_h^{n-1} + N(X)) - e^n(p^n - e^n + N(X))], \xi_e^n) - \Big(\frac{\eta_e^n - \eta_e^{n-1}}{\Delta t_c}, \xi_e^n\Big) + (\eta_e^n, \xi_e^n) \qquad (53) \\
&- (R_1(e_h^{n-1}, p_h^{n-1}, T_h^{n-1}) - R_1(e_h^n, p_h^n, T_h^n), \xi_e^n) + \Big(\frac{\hat{e}^{n-1} - \check{e}^{n-1}}{\Delta t_c}, \xi_e^n\Big) + \Big(\frac{\hat{\eta}_e^{n-1} - \check{\eta}_e^{n-1}}{\Delta t_c}, \xi_e^n\Big) \\
&+ \Big(\frac{\xi_e^{n-1} - \check{\xi}_e^{n-1}}{\Delta t_c}, \xi_e^n\Big) + \Big(\frac{\check{\eta}_e^{n-1} - \eta_e^{n-1}}{\Delta t_c}, \xi_e^n\Big) + \Big(\frac{\check{\xi}_e^{n-1} - \xi_e^{n-1}}{\Delta t_c}, \xi_e^n\Big) = \sum_{i=1}^{12} T_i.
\end{aligned}$$

The right-hand terms of (53) are considered. Applying (22) to estimate T_1

$$\left\|\phi_e\frac{\partial e}{\partial t} - \mu_e E\mathbf{u}^n\cdot e^n - \frac{e^n - \check{e}^{n-1}}{\Delta t_c}\right\| \le \Delta t_c \|\phi_e\|_{L^\infty} \int_\Omega \int_{t^{n-1}}^{t^n} \left|\frac{\partial^2 e}{\partial\tau_e^2}(\bar{Z}\check{X} + (1-\tau)X, t)\right|^2 d\tau_e dX.$$

Thus,

$$|T_1| \le K\left\|\frac{\partial^2 e}{\partial\tau_e^2}\right\|_{L^2(t^{n-1},t^n;L^2)}^2 \Delta t_c + K\left\|\xi_e^n\right\|^2. \qquad (54a)$$

Estimate T_2 by

$$|T_2| \le \|\mu_e\|_{L^\infty}\|\mathbf{u}^n - E\mathbf{u}^n\|\|\nabla e^n\|_{L^\infty}\left\|\xi_e^n\right\| \le K(\Delta t_p)^3\left\|\frac{\partial^2\mathbf{u}}{\partial t^2}\right\|_{L^2(t_{m-2},t_{m-1};L^2)}^2 + K\left\|\xi_e^n\right\|^2. \qquad (54b)$$

T_3 is bounded by

$$
\begin{aligned}
|T_3| &= \left|(e_h^n[E\mathbf{u}_h^n - \mathbf{u}^n]\cdot\nabla\mu_e + \mathbf{u}^n[e_h^n - e^n]\cdot\nabla\mu_e, \xi_e^n)\right| \\
&\le K(\Delta t_p)^3 \left\|\frac{\partial^2\mathbf{u}}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_{m-1};L^2)} + K[\,\|\psi\|^2_{L^\infty(H^{k+1})}, \|\mathbf{u}\|_{L^\infty(H^{k+1}(\mathrm{div}))}\,]h_p^{2(k+1)} \\
&+ K\|e\|_{L^\infty(H^{k+1})}\, h_c^{2(l+1)} + K\{\,\|\xi_{m-1}\|^2 + \|\xi_{m-2}\|^2 + \left\|\xi_e^n\right\|^2\}.
\end{aligned}
\tag{54c}
$$

T_4-T_7 are estimated by

$$
\begin{aligned}
&|T_4| \le K\{\left\|\xi_e^{n-1}\right\|^2 + \left\|\xi_p^{n-1}\right\|^2 + \left\|\xi_e^n\right\|^2 + (\Delta t_c)^2 + h_c^{2(l+1)}\}, \\
&|T_5| \le K(\Delta t_c)^{-1} h_c^{2(l+1)}\, \|e\|^2_{H^1(t^{n-1},t^n;H^{l+1})} + K\|\xi_e\|^2, \\
&|T_6| \le K\{\,\|\xi_e\|^2 + h_c^{2(l+1)}\}, \\
&|T_7| \le K\{\left\|\xi_e^{n-1}\right\|^2 + \left\|\xi_p^{n-1}\right\|^2 + \left\|\xi_T^{n-1}\right\|^2 + \left\|\xi_e^n\right\|^2 + h_c^{2(l+1)}\}.
\end{aligned}
\tag{54d}
$$

T_8, T_9 and T_{10} are considered in a similar manner. Let f be defined on Ω. f denotes one of the three functions, e, ξ_e or η_e. Z denotes the unit vector of $E\mathbf{u}_h^n - E\mathbf{u}^n$. Then,

$$
\begin{aligned}
\int_\Omega \frac{\hat{f}^{n-1} - \check{f}^{n-1}}{\Delta t_c}\xi_e^n dX &= (\Delta t_c)^{-1}\int_\Omega\left[\int_{\check{X}}^{\hat{X}}\frac{\partial f^{n-1}}{\partial Z}dZ\right]\xi_e^n dX \\
&= (\Delta t)^{-1}\int_\Omega\left[\int_0^1\frac{\partial f^{n-1}}{\partial Z}((1-\bar{Z})\check{X} + \bar{Z}\hat{X})d\bar{Z}\right]\left|\hat{X} - \check{X}\right|\xi_e^n dX \\
&= \int_\Omega\left[\int_0^1\frac{\partial f^{n-1}}{\partial Z}((1-\bar{Z})\check{X} + \bar{Z}\hat{X})d\bar{Z}\right]\mu_e\left|E(\mathbf{u}^n - \mathbf{u}_h^n)\right|\xi_e^n dX,
\end{aligned}
\tag{55}
$$

where $\bar{Z}\in[0,1]$ and $\hat{X} - \check{X} = \mu_e E(\mathbf{u}_h^n - \mathbf{u}^n)$. Define

$$
g_f = \int_0^1 \frac{\partial f^{n-1}}{\partial Z}((1-\bar{Z})\check{X} + \bar{Z}\hat{X})d\bar{Z}, \tag{56}
$$

then, we derive three results from (55)

$$
|T_8| \le \|\mu_e\|_{L^\infty}\|g_e\|_{L^\infty}\|E(\mathbf{u}-\mathbf{u}_h)^n\|\left\|\xi_e^n\right\|, \tag{57a}
$$

$$
|T_9| \le \|\mu_e\|_{L^\infty}\left\|g_\eta\right\|\|E(\mathbf{u}-\mathbf{u}_h)^n\|\left\|\xi_e^n\right\|_{L^\infty}, \tag{57b}
$$

$$
|T_{10}| \le \|\mu_e\|_{L^\infty}\left\|g_\xi\right\|\|E(\mathbf{u}-\mathbf{u}_h)^n\|\left\|\xi_e^n\right\|_{L^\infty}. \tag{57c}
$$

From (40) and (49), we have

$$
\|E(\mathbf{u}-\mathbf{u}_h)^n\|^2 \le K\Big\{h_p^{2(k+1)} + h_c^{2(l+1)} + \sum_{s=e,p}[\,\left\|\xi_{s,m-1}\right\|^2 + \left\|\xi_{s,m-2}\right\|^2\,]\Big\}. \tag{58}
$$

Since $g_e(X)$ is the mean value of the partial derivatives of e^{n-1}, it can be estimated by $\left\|e^{n-1}\right\|_{W^1_\infty}$. By (55a), we obtain the estimate of T_8

$$
\begin{aligned}
|T_8| &\le K\{\left\|E(\mathbf{u}^n - \mathbf{u}_h^n)\right\|^2 + \left\|\xi_e^n\right\|^2\} \\
&\le K\Big\{h_p^{2(k+1)} + h_c^{2(l+1)} + \sum_{s=e,p}[\,\left\|\xi_{s,m-1}\right\|^2 + \left\|\xi_{s,m-2}\right\|^2\,] + \left\|\xi_e^n\right\|^2\Big\}.
\end{aligned}
\tag{59}
$$

To estimate $\left\|g_\eta\right\|$ and $\left\|g_\xi\right\|$, we need to introduce the following induction hypothesis,

$$
\left\|\mathbf{U}_{h,m-i}\right\|_\infty \le \Big[\frac{h_p}{\Delta t_c}\Big]^{1/2},\; i = 1,2. \tag{60}
$$

Noting that

$$
\left\|g_f\right\|^2 \le \int_0^1\int_\Omega\Big[\frac{\partial f^{n-1}}{\partial Z}((1-\bar{Z})\check{X} + \bar{Z}\hat{X})\Big]^2 dX d\bar{Z}, \tag{61}
$$

and defining the transformation

$$G_{\bar{Z}}(X) = (1-\bar{Z})\check{X} + \bar{Z}\hat{X} = X - \mu_e[E\mathbf{u}^n(X) - \bar{Z}E(\mathbf{u}_h^n - \mathbf{u}^n)(X)]\Delta t_c, \tag{62}$$

from (61), we have

$$\left\|g_f\right\|^2 \leq \int_0^1 \sum_{\mathcal{J}} \left|\frac{\partial f^{n-1}}{\partial Z}(G_{\bar{Z}}(X))\right|^2 dXd\bar{Z}, \tag{63}$$

where $\mathcal{J}$ is a partition element of the potential equation. Using (60), we get

$$\left|\nabla E\mathbf{u}_h^n\right|_{L^\infty} \Delta t_c \leq Kh_p^{-1}\left\|\mathbf{u}_{h,m-i}\right\|_{L^\infty}\Delta t_c \leq K[\frac{\Delta t_c}{h_p}]^{1/2}. \tag{64}$$

Note that $\Delta t_c = o(h_p)$, then

$$\mathrm{detDG}_{\bar{Z}} = 1 + \mathrm{o}(1).$$

It follows from (63),

$$\left\|g_f\right\|^2 \leq K\left\|\nabla f^{n-1}\right\|^2. \tag{65}$$

Therefore,

$$\begin{aligned}
|T_9| &\leq K\left\|\nabla\eta_e^{n-1}\right\|\cdot\left\|E(\mathbf{u}^n-\mathbf{u}_h^n)\right\|\cdot(1+\ln h_c^{-1})^{2/3}h_c^{-1/2}\left\|\nabla\xi_e^n\right\| \\
&\leq Kh_c^{2l-1}h_c^{-1}(1+\ln h_c^{-1})^{4/3}\left\|E(\mathbf{u}^n-\mathbf{u}_h^n)\right\|^2 + \varepsilon\left\|\nabla\xi_e^n\right\|^2 \\
&\leq K\left\|E(\mathbf{u}^n-\mathbf{u}_h^n)\right\|^2 + \varepsilon\left\|\nabla\xi_e^n\right\|^2, && \text{(66a)} \\
|T_{10}| &\leq K\left\|\nabla\xi_e^{n-1}\right\|\cdot\left\|E(\mathbf{u}^n-\mathbf{u}_h^n)\right\|\cdot(1+\ln h_c^{-1})^{2/3}h_c^{-1/2}\left\|\nabla\xi_e^n\right\| \\
&\leq \varepsilon\{\left\|\nabla\xi_e^{n-1}\right\|^2 + \left\|\nabla\xi_e^n\right\|^2\}. && \text{(66b)}
\end{aligned}$$

To complete the proof, we need show that $\left\|\xi_{e,m-i}\right\| = O(h_p^{k+1} + h_c^{l+1} + \Delta t_c + (\Delta t_p^1)^{3/2} + (\Delta t_p)^2)$. From the discussions (Ewing, 1984; Russell, 1980) and (50), it holds obviously that $\left\|E(\mathbf{u}^n - \mathbf{u}_h^n)\right\| = o((1+\ln h_c^{-1})^{2/3}h_c^{-1/2})$. Then (66b) is obtained.

Considering (59) and (66) together,

$$\begin{aligned}
|T_8| + |T_9| + |T_{10}| \leq K\Big\{&h_p^{2(k+1)} + h_c^{2(l+1)} + (\Delta t_c)^2 + (\Delta t_p^1)^3 + (\Delta t_p)^4 \\
&+ \sum_{s=e,p}[\left\|\xi_{s,m-1}\right\|^2 + \left\|\xi_{s,m-2}\right\|^2] + \left\|\nabla\xi_e^n\right\|^2\Big\} + \varepsilon\{\left\|\nabla\xi_e^{n-1}\right\|^2 + \left\|\nabla\xi_e^n\right\|^2\}.
\end{aligned} \tag{67}$$

Applying the negative norm estimates (Ewing, 1984; Russell, 1980) for T_{11}, T_{12}, we have

$$|T_{11}| \leq Kh_c^{2(l+1)} + \varepsilon\left\|\xi_e^n\right\|_1^2, \tag{68a}$$

$$|T_{12}| \leq K\left\|\xi_e^{n-1}\right\|^2 + \varepsilon\left\|\xi_e^n\right\|_1^2. \tag{68b}$$

Using (54), (67) and (68), we rewrite (53) as

$$\begin{aligned}
&\frac{1}{2\Delta t_c}\{\left\|\xi_e^n\right\|^2 - \left\|\xi_e^{n-1}\right\|^2\} + (D_e\nabla\xi_e^n, \nabla\xi_e^n) \\
&\leq K(\|e\|_{L^\infty(H^{k+1})})h_c^{2(l+1)} + K\|e\|_{H^1(t^{n-1},t^n;H^{l+1})}h_c^{2(l+1)}(\Delta t_c)^{-1} \\
&+ K(\|\psi\|_{L^2(H^{k+1})}, \|\mathbf{u}\|_{L^\infty(H^{k+1}(\mathrm{div}))})h_p^{2(k+1)} + K\left\|\frac{\partial^2 e}{\partial\tau_e^2}\right\|^2_{L^2(t^{n-1},t^n;L^2)}\Delta t_c + K\left\|\frac{\partial^2\mathbf{u}}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_m;L^2)}(\Delta t_p)^3 \\
&+ K\Big\{\left\|\nabla\xi_e^n\right\|^2 + \sum_{s=e,p,T}\left\|\xi_s^{n-1}\right\|^2 + \sum_{s=e,p}[\left\|\xi_{s,m-1}\right\|^2 + \left\|\xi_{s,m-2}\right\|^2]\Big\} + \varepsilon\{\left\|\nabla\xi_e^{n-1}\right\|^2 + \left\|\nabla\xi_e^n\right\|^2\}.
\end{aligned} \tag{69}$$

Similarly, the hole concentration is estimated. Subtracting (35) ($t = t^n$) from (44b), we get its error equation

$$\begin{aligned}
&\frac{1}{2\Delta t_c}\{\|\xi_p^n\|^2 - \|\xi_p^{n-1}\|^2\} + (D_p\nabla\xi_p^n, \nabla\xi_p^n) \\
&\le \Big([\frac{\partial p^n}{\partial t} + \mu_p E\mathbf{u}^n\cdot\nabla p^n] - \frac{p^n - \check{p}^{n-1}}{\Delta t_c}, \xi_p^n\Big) - (\mu_p[\mathbf{u} - E\mathbf{u}^n]\cdot\nabla p^n, \xi_p^n) - ([p_h^n E\mathbf{u}_h^n - p^n\mathbf{u}^n]\cdot\nabla\mu_p, \xi_p^n) \\
&- \alpha(\mu_p[p_h^n(p_h^{n-1} - e_h^{n-1} + N(X)) - p^n(p^n - e^n + N(X))], \xi_p^n) - \Big(\frac{\eta_p^n - \eta_p^{n-1}}{\Delta t_c}, \xi_p^n\Big) + (\eta_p^n, \xi_p^n) \\
&- (R_2(e_h^{n-1}, p_h^{n-1}, T_h^{n-1}) - R_2(e_h^n, p_h^n, T_h^n), \xi_p^n) + \Big(\frac{\hat{p}^{n-1} - \check{p}^{n-1}}{\Delta t_c}, \xi_p^n\Big) + \Big(\frac{\hat{\eta}_p^{n-1} - \check{\eta}_p^{n-1}}{\Delta t_c}, \xi_p^n\Big) \\
&+ \Big(\frac{\xi_p^{n-1} - \check{\xi}_p^{n-1}}{\Delta t_c}, \xi_p^n\Big) + \Big(\frac{\check{\eta}_p^{n-1} - \eta_p^{n-1}}{\Delta t_c}, \xi_p^n\Big) + \Big(\frac{\check{\xi}_p^{n-1} - \xi_p^{n-1}}{\Delta t_c}, \xi_p^n\Big).
\end{aligned} \tag{70}$$

In a similar analysis, we obtain the following estimates

$$\begin{aligned}
&\frac{1}{2\Delta t_c}\{\|\xi_p^n\|^2 - \|\xi_p^{n-1}\|^2\} + (D_p\nabla\xi_p^n, \nabla\xi_p^n) \\
&\le K(\|p\|_{L^\infty(H^{l+1})})h_c^{2(l+1)} + K\|p\|_{H^1(t^{n-1},t^n;H^{l+1})}h_c^{2(l+1)}(\Delta t_c)^{-1} \\
&+ K(\|\psi\|_{L^\infty(H^{l+1})}, \|\mathbf{u}\|_{L^\infty(H^{k+1}(\mathrm{div}))})h_p^{2(k+1)} + K\left\|\frac{\partial^2 p}{\partial\tau_p^2}\right\|^2_{L^2(t^{n-1},t^n;L^2)}\Delta t_c + K\left\|\frac{\partial^2\mathbf{u}}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_m;L^2)}(\Delta t_p)^3 \\
&+ K\Big\{\|\nabla\xi_p^n\|^2 + \sum_{s=e,p,T}\|\xi_s^{n-1}\|^2 + \sum_{s=e,p}[\|\xi_{s,m-1}\|^2 + \|\xi_{s,m-2}\|^2]\Big\} + \varepsilon\{\|\nabla\xi_p^{n-1}\|^2 + \|\nabla\xi_p^n\|^2\}.
\end{aligned} \tag{71}$$

Subtracting (37) ($t = t^n$) from (44c), we get error equation of temperature

$$\begin{aligned}
&\frac{1}{2\Delta t_c}\Big\{\|\rho^{1/2}\xi_T^n\|^2 - \|\rho^{1/2}\xi_T^{n-1}\|^2\Big\} + (\nabla\xi_T^n, \nabla\xi_T^n) \\
&\le \Big(\rho\frac{\partial T^n}{\partial t} - \rho\frac{T^n - T^{n-1}}{\Delta t_c}, \xi_T^n\Big) + \Big((D_e\nabla e_h^n + \mu_e e_h^n E\mathbf{u}_h^n)\cdot E\mathbf{u}_h^n - (D_e\nabla e^n + \mu_e e^n\mathbf{u}^n)\cdot\mathbf{u}^n, \xi_T^n\Big) \\
&- \Big((D_p\nabla p_h^n - \mu_p p_h^n E\mathbf{u}_h^n)\cdot E\mathbf{u}_h^n - (D_p\nabla p^n - \mu_p p^n\mathbf{u}^n)\cdot\mathbf{u}^n, \xi_T^n\Big) - \Big(\frac{\eta_T^n - \eta_T^{n-1}}{\Delta t_c}, \xi_T^n\Big) + (\eta_T^n, \xi_T^n).
\end{aligned} \tag{72}$$

Continue,

$$\begin{aligned}
&\frac{1}{2\Delta t_c}\Big\{\|\rho^{1/2}\xi_T^n\|^2 - \|\rho^{1/2}\xi_T^{n-1}\|^2\Big\} + (\nabla\xi_T^n, \nabla\xi_T^n) \\
&\le K\|T\|_{H^1(t^{n-1},t^n;H^{l+1})}h_c^{2(l+1)}(\Delta t_c)^{-1} + K\left\|\frac{\partial^2\mathbf{u}}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_m;L^2)}(\Delta t_p)^3 + K\Big\{\sum_{s=e,p,T}\|\xi_s^n\|^2 + \sum_{s=e,p}[\|\xi_{s,m-1}\|^2 + \|\xi_{s,m-2}\|^2]\Big\}.
\end{aligned} \tag{73}$$

Considering (69), (71) and (73), we have

$$\begin{aligned}
&\frac{1}{2\Delta t_c}\Big\{\sum_{s=e,p}\|\xi_s^n\|^2 + \|\rho^{1/2}\xi_T^n\|^2 - \sum_{s=e,p}\|\xi_s^{n-1}\|^2 - \|\rho^{1/2}\xi_T^{n-1}\|^2\Big\} + \sum_{s=e,p}(D_s\nabla\xi_s^n, \xi_s^n) + (\nabla\xi_T^n, \nabla\xi_T^n) \\
&\le K\Big(\sum_{s=e,p}\|s\|_{L^\infty(H^{l+1})}\Big)h_c^{2(l+1)} + K\sum_{s=e,p,T}\|s\|_{H^1(t^{n-1},t^n;H^{l+1})}h_c^{2(l+1)}(\Delta t_c)^{-1} + K(\|\psi\|_{L^\infty(H^{l+1})}, \|\mathbf{u}\|_{L^\infty(H^{k+1}(\mathrm{div}))})h_p^{2(k+1)} \\
&+ K\sum_{s=e,p}\left\|\frac{\partial^2 s}{\partial\tau_p^2}\right\|^2_{L^2(t^{n-1},t^n;L^2)}\Delta t_c + K\left\|\frac{\partial^2\mathbf{u}}{\partial t^2}\right\|^2_{L^2(t_{m-2},t_m;L^2)}(\Delta t_p)^3 + K\sum_{s=e,p,T}[\|\nabla\xi_s^n\|^2 + \|\xi_s^{n-1}\|^2] \\
&+ K\sum_{s=e,p}[\|\xi_{s,m-1}\|^2 + \|\xi_{s,m-2}\|^2] + \varepsilon\sum_{s=e,p}[\|\nabla\xi_s^{n-1}\|^2 + \|\nabla\xi_s^n\|^2].
\end{aligned} \tag{74}$$

Multiplying both sides by $2\Delta t_c$, and using $\xi_s^0 = 0, s = e, p, T$, the partition restriction, (42), positive definite condition (C) and the Gronwall lemma, we conclude that

$$\max_n\sum_{s=e,p,T}\|\xi_s^n\|^2 + \sum_n\sum_{s=e,p,T}\|\nabla\xi_s^n\|^2\Delta t_c \le K\Big\{h_c^{2(l+1)} + h_p^{2(k+1)} + (\Delta t_c)^2 + (\Delta t_p^1)^3 + (\Delta t_p)^4\Big\}. \tag{75}$$

The theorem is proved by using (75) and (49).

The induction hypothesis (60) is verified now. If $t^n = t_m$, then we use (32) and (75) to get

$$\begin{aligned}
\left\|\mathbf{u}_{h,m}\right\|_{L^\infty} &\leq \|\Pi\mathbf{u}_m\|_{L^\infty} + \left\|\mathbf{u}_{h,m} - \Pi\mathbf{u}_m\right\|_{L^\infty} \leq Kh_p^{-1/2} + Kh_p^{3/2}\left\|\mathbf{u}_{h,m} - \Pi\mathbf{u}_m\right\| \\
&\leq Kh_p^{-1/2} + Kh_p^{3/2}\sum_{s=e,p}\left\|s_m - s_{h,m}\right\| \leq Kh_p^{-1/2} + Kh_p^{3/2}\sum_{s=e,p}\left[\,\left\|\xi_{s,m}\right\| + \left\|\eta_s^n\right\|\,\right] \\
&\leq Kh_p^{-1/2} + Kh_p^{3/2}\{h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p^1)^{3/2} + (\Delta t_p)^2\} \\
&\leq \left[\frac{h_c}{\Delta t_c}\right]^{1/2}.
\end{aligned} \tag{76}$$

Taking $\Delta t_c = o(h_p)$, we prove that (60) holds for h_p sufficiently small.

6. Conclusions and Discussions

Numerical simulation of three-dimensional semiconductor device transient behavior problem of heat conduction is discussed in this paper. A mixed finite element modified with the characteristics is prosed and convergence analysis is shown. In §1, the mathematical model is stated, and the physical background and related research are introduced. §2 the problem is stated and the notation in Sobolev space is introduced. The properties, the positive definite condition and the regular assumptions are given. In §3, The composite procedures are defined, where the potential is solved by the mixed finite element. The electric potential and the strength are computed simultaneously, and the computation of strength is improved by one order. The characteristic finite element is applied to solve the concentration equations and the heat conduction equation. The diffusion and convection are solved by the finite element and the characteristic scheme, respectively. The composite scheme can solve convection-dominated diffusion problems well because it avoids numerical dispersion and nonphysical oscillation. The temperature is computed by the finite element accurately. Some preliminaries are given in §4. Finally, an optimal error estimates in L^2-norm is given by using a priori estimates of differential equations and special techniques, the induction hypothesis and negative norm estimates.

Several interesting conclusions are obtained.
(I) A composite numerical scheme applied in numerical simulation of oil reservoir is adopted to solve the simulating semiconductor device behavior successfully. The basic work of Douglas (Douglas, 1987) on numerical simulation of semiconductor device is extended essentially.
(II) This research shows an optimal error estimates in L^2 norm, developing the work of Ewing, Russell and Wheeler on the characteristic mixed finite element method only for two-dimensional problem (Ewing, 1984; Russell, 1980) and giving a consideration of actual problem on three-dimensional region.
(III) The composite scheme and optimal error estimates in L^2-norm give theoretical and physical support of modern scientific computing, and this discussion is most valuable in modeling, analyzing the mechanism and designing software (He, 1989; Jerome, 1994; Shi, 2002; Yuan, 2009, 2013).

Acknowledgements

The authors express their deep appreciation to Prof. J. Douglas Jr, Prof. R. E. Ewing, and Prof. L. S. Jiang for their many helpful suggestions in the series of research on numerical simulation of semiconductor device in information science.

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