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An Upwind-Block-Centered Multistep Difference Method for a Semiconductor Device and Numerical Analysis

Yirang Yuan[1,*], Changfeng Li[1,2] and Huailing Song[3]

[1] *Institute of Mathematics, Shandong University, Jinan, Shandong 250100, China*
[2] *School of Economics, Shandong University, Jinan, Shandong 250100, China*
[3] *College of Mathematics and Econometrics, Hunan University, Changsha, Hunan 410082, China*

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Abstract. Numerical simulation of a three-dimensional semiconductor device is a fundamental problem in information science. The mathematical model is defined by a nonlinear system of initial-boundary problem including 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 concentration equations and heat conduction equation, and the electric field strength controls the concentrations and the temperature. The electric field potential is solved by the conservative block-centered method, and the order of the accuracy is improved by the electric potential. The concentrations and temperature are computed by the upwind block-centered multistep method, where three different numerical methods are involved. The multistep method is adopted to approximate the time derivative. The block-centered method is used to discretize the diffusion. The upwind scheme is applied to approximate the convection to avoid numerical dispersion and nonphysical oscillation. The block-centered difference simulates diffusion, concentrations, temperature, and the adjoint vector functions simultaneously. It has the local conservation of mass, which is an important nature in numerical simulation of a semiconductor device. By using the variation, energy estimates, induction hypothesis, embedding theorem and the technique of a priori estimates of differential equations, convergence of the optimal order is obtained. Numerical examples are provided to show the effectiveness and viability. This method provides a powerful tool for solving the challenging benchmark problem.

AMS subject classifications: 65M06, 65N06, 65N30, 82D37

Key words: Three-dimensional semiconductor device, upwind block-centered multistep difference, local conservation of mass, convergence analysis, numerical computation.

*Corresponding author.
Emails: yryuan@sdu.edu.cn (Y. Yuan), cfli@sdu.edu.cn (C. Li)

1 Introduction

Numerical simulation of a three-dimensional semiconductor device of heat conduction is a fundamental problem in information science. The mathematical model is defined by four nonlinear partial differential equations with initial-boundary conditions: 1) an elliptic equation for electric potential, 2) two convection-diffusion equations for electron concentration and hole concentration, 3) a heat equation for temperature. The electric potential appears within the concentration equations and heat equation, and the electric field strength controls the concentrations and the temperature. The mathematical model is formulated by a nonlinear partial differential system with initial-boundary conditions on a three-dimensional domain Ω [1–4],

$$-\Delta\psi=\alpha(p-e+N(X)), \qquad X=(x,y,z)^T\in\Omega, \quad t\in J=(0,\bar{T}], \tag{1.1a}$$

$$\frac{\partial e}{\partial t}=\nabla\cdot[D_e(X)\nabla e-\mu_e(X)e\nabla\psi]-R_1(e,p,T), \qquad (X,t)\in\Omega\times J, \tag{1.1b}$$

$$\frac{\partial p}{\partial t}=\nabla\cdot\left[D_p(X)\nabla p+\mu_p(X)p\nabla\psi\right]-R_2(e,p,T), \quad (X,t)\in\Omega\times J, \tag{1.1c}$$

$$\begin{aligned}\rho\frac{\partial T}{\partial t}-\Delta T=\Big\{&(D_p(X)\nabla p+\mu_p(X)p\nabla\psi)\\ &-(D_e(X)\nabla e-\mu_e(X)e\nabla\psi)\Big\}\cdot\nabla\psi, \quad (X,t)\in\Omega\times J.\end{aligned} \tag{1.1d}$$

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 (1.1a)-(1.1d) are bounded by two positive constants. $\alpha=q/\varepsilon$, where q and ε are positive constants and they denote the electronic load and the permittivity, respectively. U_T is the thermal voltage. The diffusion $D_s(X)$ is related to 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. It is important to consider a nonuniform partition in numerical simulation [5,6].

Initial conditions:

$$e(X,0)=e_0(X), \quad p(X,0)=p_0(X), \quad T(X,0)=T_0(X), \quad X\in\Omega, \tag{1.2}$$

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

In this paper, we concentrate on the Neumann boundary conditions:

$$\frac{\partial\psi}{\partial\gamma}\Big|_{\partial\Omega}=\frac{\partial e}{\partial\gamma}\Big|_{\partial\Omega}=\frac{\partial p}{\partial\gamma}\Big|_{\partial\Omega}=\frac{\partial T}{\partial\gamma}\Big|_{\partial\Omega}=0, \quad t\in J, \tag{1.3}$$

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

A compatibility condition is defined by

$$\int_\Omega [p-e+N]dX=0, \tag{1.4}$$

and the following condition is given to avoid the ambiguous solution

$$\int_\Omega \psi dX=0. \tag{1.5}$$

Numerical simulation of a semiconductor device can give important values and suggestions to manufacture modern semiconductor [5–8]. The sequence iteration was adopted to compute semiconductor problems by Gummel in 1964 and the new problem of numerical simulation in semiconductor device was proposed [9]. Douglas and Yuan put forward a simple and useful finite difference method for the one-dimensional and two-dimensional preliminary problems (constant coefficients and without temperature effect) and gave the application and rigorous theoretical results first [10, 11]. Yuan discussed the characteristic finite element method for variable coefficient problem in [12]. Since the diffusion only includes the electric-field strength $-\nabla\psi$, Yuan presented the mixed finite element of characteristics and gave the optimal-order errors in H^1-norm and L^2-norm [13, 14]. Considering actual conditions and the effect of the heat, Yuan discussed a characteristic finite difference method for three-dimensional semiconductor device of heat conduction on uniform partition [4].

The finite volume method [15, 16] has some advantages, such as the simplicity of the difference method, the high order of accuracy of the finite element method and the local conservation of mass, so it is an effective method to solve partial differential equations. The mixed finite element method [17–19] can solve the pressure and Darcy velocity simultaneously and can improve the accuracy by one order. The mixed element method can obtain the potential and the strength simultaneously, and the accuracy is improved by one-order [17–19]. A block-centered method that combines the above two methods was discussed in [20,21], and numerical experiments were presented in [22,23] to demonstrate the efficiency. Theoretical analysis was given for an elliptic problem in [24–26], along with a general discussion of the form of the block-centered difference method. Rui and Pan used this method to discuss numerical computation for hypotonic oil-gas flow problems in [27,28]. Yuan used the block-centered method to simulate semiconductor device problem and obtained good numerical results, while the physical conservation of mass did not hold [29, 30]. Based on the previous studies, an upwind-block-centered multistep method (UBCMM) is proposed for a three-dimensional semiconductor device of heat conduction in this paper. The potential is computed using a conservative block-centered scheme, and the accuracy is improved by one order for electric-field strength. UBCMM is applied to compute the concentrations and the temperature. The time derivatives are discretized by multiple steps. The diffusion is approximated by the block-centered differences and the convection is computed by the upwind scheme. The upwind method eliminates numerical dispersion and solves the convection-diffusion equations well. The concentrations, the temperature and the adjoint vector functions are computed simultaneously. The scheme is conservative locally because piece-wise-defined constant functions are taken as test functions. The conservative nature is important in numerical simulation of semiconductor device problems. By using the variation, energy estimates, induction hypothesis, embedding theorem and a priori estimates theory and special techniques of differential equations, we obtain optimal-order estimates. In this paper, numerical experiments are given for the general three-dimensional convection-diffusion equations, and the numerical results show the high computational efficiency and support the theoretical results. This method provides an efficient tool for solving challenging benchmark problems [2, 5–8] and gives an important suggestion in computing semiconductor problem such as numerical method, software design and actual applications.

Suppose that the problem of (1.1a)-(1.5) is regular,

$$\text{(R)}\quad \psi\in L^\infty(J;H^3(\Omega))\cap H^1(J;W^{4,\infty}(\Omega)),\quad e,p,T\in L^\infty(J;H^3(\Omega))\cap H^2(J;W^{4,\infty}(\Omega)). \tag{1.6}$$

The coefficients are supposed to be positive definite

$$\text{(C)}\quad 0<D_*\le D_\delta(X)\le D^*,\quad 0<\mu_*\le\mu_\delta(X)\le\mu^*,\quad (\delta=e,p),\quad 0<\rho_*\le\rho(X)\le\rho^*, \tag{1.7}$$

where D_*, D^*, μ_*, μ^*, ρ_* and ρ^* are positive constants. $R_1(e,p,T)$ and $R_2(e,p,T)$ are Lipschitz continuous on a ε_0-neighborhood of X, i.e., there exists $K>0$ such that for $|\varepsilon_i|\le\varepsilon_0$ $(1\le i\le 6)$

$$\begin{aligned}&\big|R_i(e(X,t)+\varepsilon_1,p(X,t)+\varepsilon_2,T(X,t)+\varepsilon_3)-R_i(e(X,t)+\varepsilon_4,p(X,t)+\varepsilon_5,T(X,t)+\varepsilon_6)\big|\\ \le{}& K\big\{|\varepsilon_1-\varepsilon_4|+|\varepsilon_2-\varepsilon_5|+|\varepsilon_3-\varepsilon_6|\big\},\quad i=1,2.\end{aligned} \tag{1.8}$$

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.

2 Notations and preliminaries

Two different partitions are given to define upwind block-centered multistep method. The potential and electric-field strength change slow during the physical process, thus their approximations are carried out on the nonuniform coarse partition with large steps. Other objection functions are computed on the refined nonuniform partition. The coarse partition is considered first.

For simplicity, to discuss three-dimensional problems, take $\Omega=\{[0,1]\}^3$, and let $\partial\Omega$ denote the boundary. Define

$$\begin{aligned}\delta_x:&\quad 0=x_{\frac12}<x_{\frac32}<\cdots<x_{N_x-\frac12}<x_{N_x+\frac12}=1,\\ \delta_y:&\quad 0=y_{\frac12}<y_{\frac32}<\cdots<y_{N_y-\frac12}<y_{N_y+\frac12}=1,\\ \delta_z:&\quad 0=z_{\frac12}<z_{\frac32}<\cdots<z_{N_z-\frac12}<z_{N_z+\frac12}=1.\end{aligned}$$

Ω is partitioned by $\delta_x\times\delta_y\times\delta_z$. For $i=1,2,\cdots,N_x$, $j=1,2,\cdots,N_y$, and $k=1,2,\cdots,N_z$, let

$$\begin{aligned}
&\Omega_{ijk}=\left\{(x,y,z)\Big|x_{i-\frac12}<x<x_{i+\frac12},\, y_{j-\frac12}<y<y_{j+\frac12},\, z_{k-\frac12}<z<z_{k+\frac12}\right\},\\
&x_i=\frac12(x_{i-\frac12}+x_{i+\frac12}),\quad y_j=\frac12(y_{j-\frac12}+y_{j+\frac12}),\quad z_k=\frac12(z_{k-\frac12}+z_{k+\frac12}),\\
&h_{x_i}=x_{i+\frac12}-x_{i-\frac12},\quad h_{y_j}=y_{j+\frac12}-y_{j-\frac12},\quad h_{z_k}=z_{k+\frac12}-z_{k-\frac12},\\
&h_{x,i+\frac12}=x_{i+1}-x_i,\quad h_{y,j+\frac12}=y_{j+1}-y_j,\quad h_{z,k+\frac12}=z_{k+1}-z_k,\\
&h_x=\max_{1\le i\le N_x}\{h_{x_i}\},\quad h_y=\max_{1\le j\le N_y}\{h_{y_j}\},\quad h_z=\max_{1\le k\le N_z}\{h_{z_k}\},\quad h_\psi=(h_x^2+h_y^2+h_z^2)^{\frac12}.
\end{aligned}$$

The partition supposed to be regular.

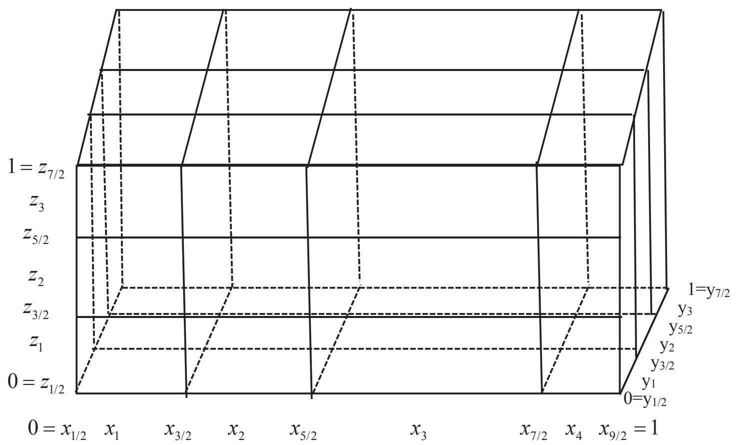

Figure 1: Nonuniform partition.

A simplified partition of $N_x=4$, $N_y=3$, and $N_z=3$ is illustrated in Fig. 1. Define an experimental space by $M_l^d(\delta_x)=\{f\in C^l[0,1]:\ f|_{\Omega_i}\in p_d(\Omega_i),\ i=1,2,\cdots,N_x\}$, where $\Omega_i=[x_{i-\frac12},x_{i+\frac12}]$ and $p_d(\Omega_i)$ denotes a space consisting of all the polynomial functions of degree at most d constricted on Ω_i. The function $f(x)$ is possibly discontinuous on $[0,1]$ if $l=-1$. $M_l^d(\delta_y)$ and $M_l^d(\delta_z)$ are defined similarly. Let

$$\begin{aligned}
&S_h=M_{-1}^0(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_{-1}^0(\delta_z),\\
&V_h=\Big\{\mathbf{w}\Big|\mathbf{w}=(w^x,w^y,w^z),w^x\in M_0^1(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_{-1}^0(\delta_z),\\
&\qquad w^y\in M_{-1}^0(\delta_x)\bigotimes M_0^1(\delta_y)\bigotimes M_{-1}^0(\delta_z),\ w^z\in M_{-1}^0(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_0^1(\delta_z),\\
&\qquad \mathbf{w}\cdot\gamma|_{\partial\Omega}=0\Big\}.
\end{aligned}$$

For a grid function $v(x,y,z)$, let v_{ijk}, $v_{i+\frac{1}{2},jk}$, $v_{i,j+\frac{1}{2},k}$ and $v_{ij,k+\frac{1}{2}}$ denote the values of $v(x_i,y_j,z_k)$, $v(x_{i+\frac{1}{2}},y_j,z_k)$, $v(x_i,y_{j+\frac{1}{2}},z_k)$ and $v(x_i,y_j,z_{k+\frac{1}{2}})$, respectively.

Define the inner products and norms by

$$(v,w)_{\bar{m}}=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_i}h_{y_j}h_{z_k}v_{ijk}w_{ijk},\qquad (v,w)_x=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_{i-\frac{1}{2}}}h_{y_j}h_{z_k}v_{i-\frac{1}{2},jk}w_{i-\frac{1}{2},jk},$$

$$(v,w)_y=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_i}h_{y_{j-\frac{1}{2}}}h_{z_k}v_{i,j-\frac{1}{2},k}w_{i,j-\frac{1}{2},k},\qquad (v,w)_z=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_i}h_{y_j}h_{z_{k-\frac{1}{2}}}v_{ij,k-\frac{1}{2}}w_{ij,k-\frac{1}{2}},$$

$$||v||_s^2=(v,v)_s,\quad s=m,x,y,z,\qquad ||v||_\infty=\max_{\substack{1\le i\le N_x,\\ 1\le j\le N_y,\\ 1\le k\le N_z}}|v_{ijk}|,$$

$$||v||_{\infty(x)}=\max_{\substack{1\le i\le N_x,\\ 1\le j\le N_y,\\ 1\le k\le N_z}}|v_{i-\frac{1}{2},jk}|,\qquad ||v||_{\infty(y)}=\max_{\substack{1\le i\le N_x,\\ 1\le j\le N_y,\\ 1\le k\le N_z}}|v_{i,j-\frac{1}{2},k}|,$$

$$||v||_{\infty(z)}=\max_{\substack{1\le i\le N_x,\\ 1\le j\le N_y,\\ 1\le k\le N_z}}|v_{ij,k-\frac{1}{2}}|.$$

For a vector $\mathbf{w}=(w^x,w^y,w^z)^T$, define its norms by

$$|||\mathbf{w}|||=\Big(||w^x||_x^2+||w^y||_y^2+||w^z||_z^2\Big)^{\frac{1}{2}},\qquad |||\mathbf{w}|||_\infty=||w^x||_{\infty(x)}+||w^y||_{\infty(y)}+||w^z||_{\infty(z)},$$

$$||\mathbf{w}||_{\bar{m}}=\big(||w^x||_{\bar{m}}^2+||w^y||_{\bar{m}}^2+||w^z||_{\bar{m}}^2\big)^{\frac{1}{2}},\qquad ||\mathbf{w}||_\infty=||w^x||_\infty+||w^y||_\infty+||w^z||_\infty.$$

Define

$$W_p^m(\Omega)=\bigg\{v\in L^p(\Omega)\bigg|\frac{\partial^n v}{\partial x^{n-l-r}\partial y^l\partial z^r}\in L^p(\Omega),\ n-l-r\ge 0,\ l=0,1,\cdots,n;$$
$$r=0,1,\cdots,n,\ n=0,1,\cdots,m;\ 0<p<\infty\bigg\}$$

and let $H^m(\Omega)=W_2^m(\Omega)$. Inner product and norm in $L^2(\Omega)$ are denoted by $(\cdot,\cdot)$ and $||\cdot||$. For a function $v\in S_h$, it clearly holds that

$$||v||_{\bar{m}}=||v||. \tag{2.1}$$

Introduce the difference operators and other notations as follows,

$$[d_xv]_{i+\frac{1}{2},jk}=\frac{v_{i+1,jk}-v_{ijk}}{h_{x,i+\frac{1}{2}}},\qquad [d_yv]_{i,j+\frac{1}{2},k}=\frac{v_{i,j+1,k}-v_{ijk}}{h_{y,j+\frac{1}{2}}},\qquad [d_zv]_{ij,k+\frac{1}{2}}=\frac{v_{ij,k+1}-v_{ijk}}{h_{z,k+\frac{1}{2}}},$$

$$[D_xw]_{ijk}=\frac{w_{i+\frac{1}{2},jk}-w_{i-\frac{1}{2},jk}}{h_{x_i}},\quad [D_yw]_{ijk}=\frac{w_{i,j+\frac{1}{2},k}-w_{i,j-\frac{1}{2},k}}{h_{y_j}},\quad [D_zw]_{ijk}=\frac{w_{ij,k+\frac{1}{2}}-w_{ij,k-\frac{1}{2}}}{h_{z_k}},$$

$$\hat{w}^x_{ijk}=\frac{w^x_{i+\frac{1}{2},jk}+w^x_{i-\frac{1}{2},jk}}{2},\qquad \hat{w}^y_{ijk}=\frac{w^y_{i,j+\frac{1}{2},k}+w^y_{i,j-\frac{1}{2},k}}{2},\qquad \hat{w}^z_{ijk}=\frac{w^z_{ij,k+\frac{1}{2}}+w^z_{ij,k-\frac{1}{2}}}{2},$$

and $\hat{\mathbf{w}}_{ijk}=(\hat{w}^x_{ijk},\hat{w}^y_{ijk},\hat{w}^z_{ijk})^T$. Let N denote a positive integer, $\Delta t_s=T/N$, $t^n=n\Delta t_s$, and let v^n denote the value at t^n, $d_tv^n=(v^n-v^{n-1})/\Delta t_s$.

Based on the above notation, several preliminary statements can be given.

Lemma 2.1. *For* $v\in S_h$, $\mathbf{w}\in V_h$,

$$(v,D_xw^x)_{\bar{m}}=-(d_xv,w^x)_x,\quad \left(v,D_yw^y\right)_{\bar{m}}=-\left(d_yv,w^y\right)_y,\quad (v,D_zw^z)_{\bar{m}}=-(d_zv,w^z)_z. \tag{2.2}$$

Lemma 2.2. *For* $\mathbf{w}\in V_h$,

$$||\hat{\mathbf{w}}||_{\bar{m}}\le|||\mathbf{w}|||. \tag{2.3}$$

Lemma 2.3. *For* $\mathbf{w}\in V_h$,

$$||w^x||_x\le||D_xw^x||_{\bar{m}},\quad ||w^y||_y\le||D_yw^y||_{\bar{m}},\quad ||w^z||_z\le||D_zw^z||_{\bar{m}}. \tag{2.4}$$

Another partition is obtained by refining the coarse partition of $\Omega=[0,1]^3$ uniformly, where the step is usually taken as $1/l$ times the coarse step, that is, $h_s=h_\psi/l$ for a positive integer l such as $l=4$. The other notation is defined as above.

3 The upwind block-centered multistep difference procedure

To apply the method of block-centered difference, the problem of (1.1a)-(1.1d) is reformulated as follows

$$\nabla\cdot\mathbf{u}=\alpha(p-e+N),\qquad X\in\Omega,\quad t\in J, \tag{3.1a}$$
$$\mathbf{u}=-\nabla\psi,\qquad X\in\Omega,\quad t\in J. \tag{3.1b}$$

The upwind block-centered multistep procedure is constructed to solve the concentration equations (1.1b), (1.1c) and the temperature equation (1.1d). The three equations should be written in the divergence forms. Let $\mathbf{g}_r=\mu_r(X)r\mathbf{u}$, $\bar{\mathbf{z}}_r=-\nabla r$, $\mathbf{z}_r=D_r\bar{\mathbf{z}}_r$, $r=e,p$ and $\mathbf{z}_T=-\nabla T$. Then,

$$\frac{\partial e}{\partial t}-\nabla\cdot\mathbf{g}_e+\nabla\cdot\mathbf{z}_e=-R_1(e,p,T),\qquad X\in\Omega,\quad t\in J, \tag{3.2a}$$
$$\frac{\partial p}{\partial t}+\nabla\cdot\mathbf{g}_p+\nabla\cdot\mathbf{z}_p=-R_2(e,p,T),\qquad X\in\Omega,\quad t\in J, \tag{3.2b}$$
$$\rho(X)\frac{\partial T}{\partial t}+\nabla\cdot\mathbf{z}_T=\left\{(\mathbf{z}_p+\mathbf{g}_p)-(\mathbf{z}_e-\mathbf{g}_e)\right\}\cdot\mathbf{u},\qquad X\in\Omega,\quad t\in J. \tag{3.2c}$$

The expanded block-centered difference is discussed in [31, 32], which can approximate the diffusion flux functions $\mathbf{z}_e$, $\mathbf{z}_p$, $\mathbf{z}_T$ and the gradient functions $\bar{\mathbf{z}}_e$, $\bar{\mathbf{z}}_p$, simultaneously.

The time-dependent partitions are defined.

(1) For the electrostatic potential, Δt_ψ is the time step and $\Delta t_{\psi,1}$ is the first time step. $J=[0,\bar{T}]$ is partitioned by $0=t_0<t_1<\cdots<t_M=\bar{T}$, and the i-th time level is denoted by $t_i=\Delta t_{\psi,1}+(i-1)\Delta t_\psi$, $i\geq 1$.

(2) For the concentrations and the temperature, it is partitioned by $0=t^0<t^1<\cdots<t^N=\bar{T}$, Δt_s is the time step and $t^n=n\Delta t_s$.

(3) Suppose that there exists a positive integer n such that $t_m=t^n$ for any m, and $\frac{\Delta t_\psi}{\Delta t_s}$ is a positive integer. Let $j^0=\Delta t_{\psi,1}/\Delta t_s$, $j=\Delta t_\psi/\Delta t_s$.

The backward difference operators are defined,

$$f^n\equiv f^n(X)\equiv f(X,t^n),\qquad \delta f^n=f^n-f^{n-1},$$
$$\delta^2 f^n=f^n-2f^{n-1}+f^{n-2},\qquad \delta^3 f^n=f^n-3f^{n-1}+3f^{n-2}-f^{n-3}.$$

Let

$$d_t f^n=\frac{\delta f^n}{\Delta t_s},\quad d_t^j f^n=\frac{\delta^j f^n}{(\Delta t_s)^j}.$$

Let Ψ, $\mathbf{U}$, E, $\mathbf{Z}_e$, $\bar{\mathbf{Z}}_e$, P, $\mathbf{Z}_p$, $\bar{\mathbf{Z}}_p$, H and $\mathbf{Z}_T$ denote numerical solutions of ψ, $\mathbf{u}$, e, $\mathbf{z}_e$, $\bar{\mathbf{z}}_e$, p, $\mathbf{z}_p$, $\bar{\mathbf{z}}_p$, T and $\mathbf{z}_T$ in $S_h\times V_h\times S_h\times V_h\times V_h\times S_h\times V_h\times V_h\times S_h\times V_h$, respectively. Using the notation and Lemmas 2.1-2.3 in Section 2, we state the block-centered scheme for the potential and electric-field strength as

$$\big(D_xU_m^x+D_yU_m^y+D_zU_m^z,v\big)_{\bar{m}}=\alpha\big(E_m^n-P_m^n+N,v\big)_{\bar{m}},\qquad \forall v\in S_h,\tag{3.3a}$$
$$\big(U_m^x,w^x\big)_x+\big(U_m^y,w^y\big)_y+\big(U_m^z,w^z\big)_z-\big(\Psi_m,D_xw^x+D_xw^y+D_xw^z\big)_{\bar{m}}=0,\qquad \mathbf{w}\in V_h.\tag{3.3b}$$

The discrete variational form of (3.2a) is

$$\begin{aligned}&\left(\frac{\partial e}{\partial t},v\right)_{\bar{m}}-\big(\nabla\cdot\mathbf{g}_e,v\big)_{\bar{m}}+\big(\nabla\cdot\mathbf{z}_e,v\big)_{\bar{m}}\\&=-\big(R_1(e,p,T),v\big)_{\bar{m}},&&\forall v\in S_h,&(3.4a)\\&\big(\bar{Z}_e^x,w^x\big)_x+\big(\bar{Z}_e^y,w^y\big)_y+\big(\bar{Z}_e^z,w^z\big)_z\\&=\big(e,D_xw^x+D_xw^y+D_xw^z\big)_{\bar{m}}=0,&&\mathbf{w}\in V_h,&(3.4b)\\&\big(Z_e^x,w^x\big)_x+\big(Z_e^y,w^y\big)_y+\big(Z_e^z,w^z\big)_z\\&=\big(D_e\bar{Z}_e^x,w^x\big)_x+\big(D_e\bar{Z}_e^y,w^y\big)_y+\big(D_e\bar{Z}_e^z,w^z\big)_z,&&\mathbf{w}\in V_h.&(3.4c)\end{aligned}$$

The upwind block-centered multistep procedure is given for the electron concentration equation (3.4). Given initial approximation $\{E^i\in S_h,\ i=0,1,\cdots,\mu-1\}$, numerical solutions of $E^n\in S_h$, $\bar{\mathbf{Z}}_e^n\in V_h$ and $\mathbf{Z}_e^n\in V_h$ are defined by

$$\sum_{j=1}^{\mu}\frac{\Delta t_s^{j-1}}{j}d_t^jE^n-\nabla\cdot\mathbf{G}_e^n+\nabla\cdot\mathbf{Z}_e^n=-R_1(E^n,P^n,H^n),\quad (n=\mu,\mu+1,\cdots,N).\tag{3.5}$$

Table 1: The values of the parameters ($\mu=1,2,3$).

μ	$\beta(\mu)$	$\alpha_1(\mu)$	$\alpha_2(\mu)$	$\hat{E}(\mu)f^n$
1	1	0	0	$f^n-\delta f^n$
2	2/3	1/3	0	$f^n-\delta^2 f^n$
3	6/11	7/11	−2/11	$f^n-\delta^3 f^n$

In order to compute E^n accurately, the values of E^j ($j=0,1,\cdots,\mu-1$) are determined by a single program. They approximate e^j with the accuracy of μ-th order.

For simplicity, we consider three cases, $\mu=1,2,3$, then the variation of (3.5) is defined by

$$\begin{aligned}&\left(\frac{E^n-E^{n-1}}{\Delta t_s},v\right)_{\bar{m}}-\beta(\mu)\left(\nabla\cdot\mathbf{G}_e^n,v\right)_{\bar{m}}+\beta(\mu)\left(\nabla\cdot\mathbf{Z}_e^n,v\right)_{\bar{m}}\\=&\frac{1}{\Delta t_s}\left(\alpha_1(\mu)\delta E^{n-1}+\alpha_2(\mu)\delta E^{n-2}],v\right)_{\bar{m}}-\beta(\mu)\left(R_1(\hat{E}(\mu)(E,P,H)^n),v\right)_{\bar{m}},\quad\forall v\in S_h.\end{aligned}\tag{3.6}$$

The values of $\alpha_i(\mu)$, $\beta(\mu)$, $\hat{E}(\mu)f^n$ are computed by (3.5), illustrated in Table 1 for μ=1,2,3.

The scheme of $\mu=1$ is the upwind block-centered difference method. In this paper, we consider the case of $\mu=2$ to interpret the multistep method. The scheme is

$$\begin{aligned}&\left(\frac{E^n-E^{n-1}}{\Delta t_s},v\right)_{\bar{m}}-\frac{2}{3}\left(\nabla\cdot\mathbf{G}_e^n,v\right)_{\bar{m}}+\frac{2}{3}\left(\sum_{s=x,y,z}D_sZ_e^{s,n},v\right)_{\bar{m}}\\=&\frac{1}{\Delta t_s}\left(\frac{1}{3}\delta E^{n-1},v\right)_{\bar{m}}-\frac{2}{3}\left(R_1(\hat{E}(2)(E,P,H)^n),v\right)_{\bar{m}},\qquad\forall v\in S_h,\end{aligned}\tag{3.7a}$$

$$\left(\bar{Z}_e^{x,n},w^x\right)_x+\left(\bar{Z}_e^{y,n},w^y\right)_y+\left(\bar{Z}_e^{z,n},w^z\right)_z=\left(E^n,\sum_{s=x,y,z}D_sw^s\right)_{\bar{m}},\qquad\mathbf{w}\in V_h,\tag{3.7b}$$

$$\left(Z_e^{x,n},w^x\right)_x+\left(Z_e^{y,n},w^y\right)_y+\left(Z_e^{z,n},w^z\right)_z=\sum_{s=x,y,z}\left(D_e\bar{Z}_e^{s,n},w^s\right)_s,\qquad\mathbf{w}\in V_h.\tag{3.7c}$$

In (3.7a), $\hat{E}(2)\mathbf{U}^n$ is defined by

$$\hat{E}(2)\mathbf{U}^n=\bar{E}\mathbf{U}^n-\delta^2\bar{E}\mathbf{U}^n.$$

The value $\bar{E}\mathbf{U}^n$ at t^n, $t_{m-1}<t^n\le t_m$, is assigned by an extrapolation

$$\bar{E}\mathbf{U}^n=\begin{cases}\mathbf{U}_0, & t_0<t^n\le t_1,\quad m=1,\\ \left(1+\dfrac{t^n-t_{m-1}}{t_{m-1}-t_{m-2}}\right)\mathbf{U}_{m-1}-\dfrac{t^n-t_{m-1}}{t_{m-1}-t_{m-2}}\mathbf{U}_{m-2}, & t_{m-1}<t^n\le t_m,\quad m\ge 2.\end{cases}\tag{3.8}$$

An upwind approximation flux $\mathbf{G}_e$ is computed by using E. The value of $\mathbf{G}_e^n$ is defined as follows. The mean value of integral of $\mathbf{G}_e^n\cdot\gamma$ is supposed to be zero because of $\mathbf{g}_e=\mu_e e\mathbf{u}=0$

on $\partial\Omega$. Let σ denote the shared plane of ω_1 and ω_2. x_l is the barycentre and γ_l is the unit outer normal vector to ω_2. Define

$$\mathbf{G}_e^n\cdot\gamma_l=\begin{cases} E_{\omega_1}^n(\mu_e\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l), & (\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l)\geq 0,\\ E_{\omega_2}^n(\mu_e\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l), & (\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l)<0,\end{cases}$$

where $E_{\omega_1}^n$ and $E_{\omega_2}^n$ denote the values of E^n on ω_1 and ω_2, respectively. Then, we can assign the value of $\mathbf{G}_e^n$.

Similarly, (3.2b) is solved by an upwind-block-centered multistep method. If $\{P^i\in S_h,\ i=0,1,\cdots,\mu-1\}$ is given, then $P^n\in S_h$, $\bar{\mathbf{Z}}_p^n\in V_h$ and $\mathbf{Z}_p^n\in V_h$ are defined by

$$\sum_{j=1}^{\mu}\frac{\Delta t_s^{j-1}}{j}d_t^jP^n+\nabla\cdot\mathbf{G}_p^n+\nabla\cdot\mathbf{Z}_p^n=-R_2(E^n,P^n,H^n),\quad (n=\mu,\mu+1,\cdots,N). \tag{3.9}$$

The procedures are formulated as follows for $\mu=2$

$$\begin{aligned}&\Big(\frac{P^n-P^{n-1}}{\Delta t_s},v\Big)_{\bar{m}}+\frac{2}{3}\Big(\nabla\cdot\mathbf{G}_p^n,v\Big)_{\bar{m}}+\frac{2}{3}\Big(\sum_{s=x,y,z}D_sZ_p^{s,n},v\Big)_{\bar{m}}\\ &=\frac{1}{\Delta t_s}\Big(\frac{1}{3}\delta P^{n-1},v\Big)_{\bar{m}}-\frac{2}{3}\big(R_2(\hat{E}(2)(E,P,H)^n),v\big)_{\bar{m}}, \qquad \forall v\in S_h,\end{aligned} \tag{3.10a}$$

$$\big(\bar{Z}_p^{x,n},w^x\big)_x+\big(\bar{Z}_p^{y,n},w^y\big)_y+\big(\bar{Z}_p^{z,n},w^z\big)_z=\Big(P^n,\sum_{s=x,y,z}D_sw^s\Big)_{\bar{m}}, \qquad \mathbf{w}\in V_h, \tag{3.10b}$$

$$\big(Z_p^{x,n},w^x\big)_x+\big(Z_p^{y,n},w^y\big)_y+\big(Z_p^{z,n},w^z\big)_z=\sum_{s=x,y,z}\big(D_p\bar{Z}_p^{s,n},w^s\big)_s, \qquad \mathbf{w}\in V_h. \tag{3.10c}$$

The approximation of $\mathbf{G}_p^n$ is defined by

$$\mathbf{G}_p^n\cdot\gamma_l=\begin{cases} E_{\omega_1}^n(\mu_p\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l), & (\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l)\geq 0,\\ E_{\omega_2}^n(\mu_p\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l), & (\hat{E}(2)\mathbf{U}^n\cdot\gamma_l)(x_l)<0.\end{cases}$$

The heat equation (3.2c) is solved by a similar block-centered multistep scheme. If $\{H^i\in S_h,\ i=0,1,\cdots,\mu-1\}$ is given, then $H^n\in S_h$ and $\mathbf{Z}_T^n\in V_h$ are computed by

$$\sum_{j=1}^{\mu}\frac{\Delta t_s^{j-1}}{j}d_t^jH^n+\nabla\cdot\mathbf{Z}_T^n=\big\{(\mathbf{Z}_p^{n-1}+\mu_pP^{n-1}\bar{E}\mathbf{U}^n)-(\mathbf{Z}_e^{n-1}-\mu_eE^{n-1}\bar{E}\mathbf{U}^n)\big\}\cdot\bar{E}\mathbf{U}^n. \tag{3.11}$$

For $\mu=2$, the procedures are expressed by

$$\begin{aligned}&\Big(\frac{H^n-H^{n-1}}{\Delta t_s},v\Big)_{\bar{m}}+\frac{2}{3}\Big(\sum_{s=x,y,z}D_sZ_T^{s,n},v\Big)_{\bar{m}}\\ &=\frac{1}{\Delta t_s}\big(\frac{1}{3}\delta H^{n-1},v\big)_{\bar{m}}+\frac{2}{3}\big([(\mathbf{Z}_p^{n-1}+\mu_pP^{n-1}\bar{E}\mathbf{U}^n)\\ &\quad-(\mathbf{Z}_e^{n-1}-\mu_eE^{n-1}\bar{E}\mathbf{U}^n)]\cdot\bar{E}\mathbf{U}^n,v\big)_{\bar{m}}, \qquad \forall v\in S_h,\end{aligned} \tag{3.12a}$$

$$\left(Z_T^{x,n},w^x\right)_x+\left(Z_T^{y,n},w^y\right)_y+\left(Z_T^{z,n},w^z\right)_z=\left(H^n,\sum_{s=x,y,z}D_s w^s\right)_{\bar{m}},\qquad \mathbf{w}\in V_h. \tag{3.12b}$$

The upwind block-centered multistep scheme of (3.3), (3.7), (3.10) and (3.12) runs as follows to solve the problem of (1.1a)-(1.5). First, (E^0,E^1), (P^0,P^1) and (H^0,H^1) are determined by using initial conditions, then $\{\mathbf{U}_0,\Psi_0\}$ is obtained from (3.3a) and (3.3b). Second, $(E^2,P^2,H^2),(E^3,P^3,H^3),\cdots,(E^{j_0},P^{j_0},H^{j_0})$ are computed by using the procedures of (3.7), (3.10) and (3.12). Let

$$E^{j_0+(m-1)j}=E_m,\quad P^{j_0+(m-1)j}=P_m,\quad H^{j_0+(m-1)j}=H_m.$$

From (3.3), we can obtain $\{\mathbf{U}_m,\Psi_m\}$. Third, the computations are repeated for $n\geq 2$ and $m\geq 1$. The values of $(E^{j_0+(m-1)j+1},P^{j_0+(m-1)j+1},H^{j_0+(m-1)j+1})$, $(E^{j_0+(m-1)j+2},P^{j_0+(m-1)j+2},H^{j_0+(m-1)j+2})$, $\cdots$, $(E^{j_0+mj},P^{j_0+mj},H^{j_0+mj})$ are obtained. Finally, we can get all the numerical solutions. According to (C), numerical solutions exist and are unique.

Remark 3.1. Multi-step method requires the values of $(E^0,P^0,H^0),(E^1,P^1,H^1),\cdots,(E^{\mu-1},P^{\mu-1},H^{\mu-1})$, and it is expected that these values are computed with a local truncation error of μ-th order. When μ is small, we can adopt the following techniques

(1) Using the Crank-Nicolson method;

(2) Using a sufficiently small step compared with Δt_s.

4 The principle of mass conservation

Suppose that the recombination rates are zero, $R_i(e,p,T)\equiv 0$, $i=1,2$, and suppose that the Neumann boundary condition is homogeneous. Then the local conservation of mass on an element $\omega\in\Omega$,

$$\omega=\omega_{ijk}=[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}]\times[y_{j-\frac{1}{2}},y_{j+\frac{1}{2}}]\times[z_{k-\frac{1}{2}},z_{k+\frac{1}{2}}]$$

is interpreted by

$$\int_\omega \frac{\partial e}{\partial t}dX+\int_{\partial\omega}\mathbf{g}_e\cdot\gamma_{\partial\omega}ds-\int_{\partial\omega}\mathbf{z}_e\cdot\gamma_{\partial\omega}ds=0, \tag{4.1a}$$

$$\int_\omega \frac{\partial p}{\partial t}dX-\int_{\partial\omega}\mathbf{g}_p\cdot\gamma_{\partial\omega}ds-\int_{\partial\omega}\mathbf{z}_p\cdot\gamma_{\partial\omega}ds=0. \tag{4.1b}$$

Here ω denotes an element of the partition of Ω for the concentration, $\partial\omega$ is the boundary of ω, and $\gamma_{\partial\omega}$ is the unit outer normal vector. The multistep schemes of (3.7a) and (3.10a) have the following nature.

Theorem 4.1. *If* $R_i(e,p,T)\equiv 0$, $i=1,2$, *then*

$$\int_\omega \frac{E^n-E^{n-1}}{\Delta t_s}dX-\frac{1}{3}\int_{\partial\omega}\frac{E^{n-1}-E^{n-2}}{\Delta t_s}dX+\frac{2}{3}\int_{\partial\omega}\mathbf{G}_e^n\cdot\gamma_{\partial\omega}ds-\frac{2}{3}\int_{\partial\omega}\mathbf{Z}_e^n\cdot\gamma_{\partial\omega}ds=0, \tag{4.2a}$$

$$\int_\omega \frac{P^n-P^{n-1}}{\Delta t_s}dX-\frac{1}{3}\int_{\partial\omega}\frac{P^{n-1}-P^{n-2}}{\Delta t_s}dX-\frac{2}{3}\int_{\partial\omega}\mathbf{G}_p^n\cdot\gamma_{\partial\omega}ds-\frac{2}{3}\int_{\partial\omega}\mathbf{Z}_p^n\cdot\gamma_{\partial\omega}ds=0. \tag{4.2b}$$

Proof. We only prove (4.2a). The proof of (4.2b) can be finished in a similar manner. For a function $v\in S_h$, its value is assigned by 1 on $\omega=\Omega_{ijk}$ and 0 on other elements, i.e.,

$$v(X_{ijk})=\begin{cases} 1, & \omega,\\ 0, & \text{otherwise.}\end{cases}$$

Then (3.7a) is rewritten as

$$\begin{aligned}&\Big(\frac{E^n-E^{n-1}}{\Delta t_s},1\Big)_{\Omega_{ijk}}-\frac{1}{3}\Big(\frac{E^{n-1}-E^{n-2}}{\Delta t_s},1\Big)_{\Omega_{ijk}}+\frac{2}{3}\int_{\partial\Omega_{ijk}}\mathbf{G}_e^n\cdot\gamma_{\partial\omega}ds\\ &\quad+\frac{2}{3}\big(D_xZ_e^{x,n}+D_yZ_e^{y,n}+D_zZ_e^{z,n},1\big)_{\Omega_{ijk}}=0.\end{aligned} \tag{4.3}$$

Using the notation in Section 2,

$$\Big(\frac{E^n-E^{n-1}}{\Delta t_s},1\Big)_{\omega_{ijk}}=\sum_{i,j,k}\Big(\frac{E^n_{ijk}-E^{n-1}_{ijk}}{\Delta t_s}\Big)h_{x_i}h_{y_j}h_{z_k}=\int_\omega\frac{E^n-E^{n-1}}{\Delta t_s}dX, \tag{4.4a}$$

$$-\frac{1}{3}\Big(\frac{E^{n-1}-E^{n-2}}{\Delta t_s},1\Big)_{\omega_{ijk}}=-\frac{1}{3}\int_\omega\frac{E^{n-1}-E^{n-2}}{\Delta t_s}dX, \tag{4.4b}$$

$$\begin{aligned}\frac{2}{3}\Big(\sum_{s=x,y,z}D_sZ_e^{s,n},1\Big)_{\omega_{ijk}}&=\frac{2}{3}\sum_{j,k}\big(Z^{x,n}_{e,i+\frac12,jk}-Z^{x,n}_{e,i-\frac12,jk}\big)h_{y_j}h_{z_k}+\frac{2}{3}\sum_{i,k}\big(Z^{y,n}_{e,i,j+\frac12,k}-Z^{y,n}_{e,i,j-\frac12,k}\big)h_{x_i}h_{z_k}\\ &\quad+\frac{2}{3}\sum_{i,j}\big(Z^{z,n}_{e,ij,k+\frac12}-Z^{z,n}_{e,i,j-\frac12,k}\big)h_{x_i}h_{y_j}=-\frac{2}{3}\int_{\partial\omega}\mathbf{Z}_e^n\cdot\gamma_{\partial\omega}ds.\end{aligned} \tag{4.4c}$$

Substituting (4.4) into (4.3), we complete the proof. □

Furthermore, we conclude the conservation on the whole domain.

Theorem 4.2. *If* $R_i(e,p,T)\equiv 0$, $i=1,2$ *and the homogeneous Neumann boundary condition holds, then* (3.3a) *and* (3.7a) *have the following nature*

$$\int_\Omega\frac{E^n-E^{n-1}}{\Delta t_s}dX-\frac{1}{3}\int_\Omega\frac{E^{n-1}-E^{n-2}}{\Delta t_s}dX=0,\qquad n>0, \tag{4.5a}$$

$$\int_\Omega\frac{P^n-P^{n-1}}{\Delta t_s}dX-\frac{1}{3}\int_\Omega\frac{P^{n-1}-P^{n-2}}{\Delta t_s}dX=0,\qquad n>0. \tag{4.5b}$$

Proof. (4.5a) is proved first. (4.5b) can be discussed similarly. Summing (4.2a) on all the elements, we have

$$\begin{aligned}&\sum_{\omega}\int_{\omega}\frac{E^n-E^{n-1}}{\Delta t_s}dX-\frac{1}{3}\sum_{\omega}\int_{\partial\omega}\frac{E^{n-1}-E^{n-2}}{\Delta t_s}dX\\&\quad+\frac{2}{3}\sum_{\omega}\int_{\partial\omega}\mathbf{G}_e^n\cdot\gamma_{\partial\omega}ds-\frac{2}{3}\sum_{\omega}\int_{\partial\omega}\mathbf{Z}_e^n\cdot\gamma_{\partial\omega}ds=0.\end{aligned}\tag{4.6}$$

ω_1 intersects ω_2 at σ. x_l is the barycentre and γ_l is the unit outer normal vector to ω_2. By the definition of convection flux, if $\bar{E}(2)\mathbf{U}^n\cdot\gamma_l(X)\geq 0$ on ω_1, then

$$\int_{\sigma_l}\mathbf{G}_e^n\cdot\gamma_l ds=E_{\omega_1}^n\bar{E}(2)\mathbf{U}^n\cdot\gamma_l(X)|\sigma_l|,\tag{4.7a}$$

where $|\sigma_l|$ is the measure of σ_l. On ω_2, the unit normal vector to σ_l is $-\gamma_l$, and $\bar{E}(2)\mathbf{U}^n\cdot(-\gamma_l(X))\leq 0$. Then,

$$\int_{\sigma_l}\mathbf{G}_e^n\cdot(-\gamma_l)ds=-E_{\omega_1}^n\bar{E}(2)\mathbf{U}^n\cdot\gamma_l(X)|\sigma_l|.\tag{4.7b}$$

The signs of (4.7a) and (4.7b) are contrary, therefore,

$$\frac{2}{3}\sum_{\omega}\int_{\partial\omega}\mathbf{G}_e^n\cdot\gamma_{\partial\omega}ds=0.\tag{4.8}$$

Similarly, we have

$$-\frac{2}{3}\sum_{\omega}\int_{\partial\omega}\mathbf{Z}_e^n\cdot\gamma_{\partial\omega}ds=-\frac{2}{3}\int_{\partial\Omega}\mathbf{Z}_e^n\cdot\gamma_{\partial\Omega}ds=0.\tag{4.9}$$

Substituting (4.8) and (4.9) into (4.6), we complete the proof of (4.5a). □

The conservation nature is important in the numerical simulation of semiconductor device.

5 Convergence analysis

Elliptic projections are introduced first for convergence analysis. Define $\tilde{\mathbf{U}}\in V_h$ and $\tilde{\Psi}\in S_h$ by

$$\big(D_x\tilde{U}_m^x+D_y\tilde{U}_m^y+D_z\tilde{U}_m^z,v\big)_{\bar{m}}=\alpha\big(e_m-p_m+N,v\big)_{\bar{m}},\qquad\forall v\in S_h,\tag{5.1a}$$

$$\big(\tilde{U}_m^x,w^x\big)_x+\big(\tilde{U}_m^y,w^y\big)_y+\big(\tilde{U}_m^z,w^z\big)_z=\big(\tilde{\Psi}_m,D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}},\qquad\forall\mathbf{w}\in V_h,\tag{5.1b}$$

where e and p are the exact solutions of (1.1a)-(1.5). Let

$$F_e=R_1(e,p,T)-\left(\frac{\partial e}{\partial t}-\nabla\cdot\mathbf{g}_e\right).$$

Define $\tilde{\mathbf{Z}}_e,\tilde{\tilde{\mathbf{Z}}}_e\in V_h$ and $\tilde{E}\in S_h$ by

$$\big(D_x\tilde{Z}_e^x+D_y\tilde{Z}_e^y+D_z\tilde{Z}_e^z,v\big)_{\bar{m}}=\big(F_e,v\big)_{\bar{m}},\qquad \forall v\in S_h, \tag{5.2a}$$

$$\big(\tilde{\tilde{Z}}_e^x,w^x\big)_x+\big(\tilde{\tilde{Z}}_e^y,w^y\big)_y+\big(\tilde{\tilde{Z}}_e^z,w^z\big)_z=\big(\tilde{E},D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}},\qquad \forall \mathbf{w}\in V_h, \tag{5.2b}$$

$$\big(\tilde{Z}_e^x,w^x\big)_x+\big(\tilde{Z}_e^y,w^y\big)_y+\big(\tilde{Z}_e^z,w^z\big)_z=\big(D_e\tilde{\tilde{Z}}_e^x,w^x\big)_x+\big(D_e\tilde{\tilde{Z}}_e^y,w^y\big)_y+\big(D_e\tilde{\tilde{Z}}_e^z,w^z\big)_z,\qquad \forall \mathbf{w}\in V_h. \tag{5.2c}$$

Let

$$F_p=R_2(e,p,T)-\left(\frac{\partial p}{\partial t}+\nabla\cdot\mathbf{g}_p\right).$$

Define $\tilde{\mathbf{Z}}_p,\tilde{\tilde{\mathbf{Z}}}_p\in V_h$ and $\tilde{P}\in S_h$ by

$$\big(D_x\tilde{Z}_p^x+D_y\tilde{Z}_p^y+D_z\tilde{Z}_p^z,v\big)_{\bar{m}}=\big(F_p,v\big)_{\bar{m}},\qquad \forall v\in S_h, \tag{5.3a}$$

$$\big(\tilde{\tilde{Z}}_p^x,w^x\big)_x+\big(\tilde{\tilde{Z}}_p^y,w^y\big)_y+\big(\tilde{\tilde{Z}}_p^z,w^z\big)_z=\big(\tilde{P},D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}},\qquad \forall \mathbf{w}\in V_h, \tag{5.3b}$$

$$\big(\tilde{Z}_p^x,w^x\big)_x+\big(\tilde{Z}_p^y,w^y\big)_y+\big(\tilde{Z}_p^z,w^z\big)_z=\big(D_p\tilde{\tilde{Z}}_p^x,w^x\big)_x+\big(D_p\tilde{\tilde{Z}}_p^y,w^y\big)_y+\big(D_p\tilde{\tilde{Z}}_p^z,w^z\big)_z,\qquad \forall \mathbf{w}\in V_h. \tag{5.3c}$$

Let

$$F_T=\big\{(\mathbf{z}_p+\mathbf{g}_p)-(\mathbf{z}_e-\mathbf{g}_e)\big\}\cdot\mathbf{u}-\rho\frac{\partial T}{\partial t}.$$

Define $\tilde{\mathbf{Z}}_T\in V_h$ and $\tilde{H}\in S_h$ by

$$\big(D_x\tilde{Z}_T^x+D_y\tilde{Z}_T^y+D_z\tilde{Z}_T^z,v\big)_{\bar{m}}=\big(F_T,v\big)_{\bar{m}},\qquad \forall v\in S_h, \tag{5.4a}$$

$$\big(\tilde{Z}_T^x,w^x\big)_x+\big(\tilde{Z}_T^y,w^y\big)_y+\big(\tilde{Z}_T^z,w^z\big)_z=\big(\tilde{H},D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}},\qquad \forall \mathbf{w}\in V_h. \tag{5.4b}$$

Let

$$\begin{aligned}
&\pi=\Psi-\tilde{\Psi}, && \eta=\tilde{\Psi}-\psi, && \sigma=\mathbf{U}-\tilde{\mathbf{U}}, && \rho_T=\tilde{\mathbf{U}}-\mathbf{u},\\
&\xi_s=S-\tilde{S}, && \zeta_s=\tilde{S}-s\ \ (s=e,p), && \xi_T=H-\tilde{H}, && \zeta_T=\tilde{H}-T,\\
&\alpha_{z,s}=\mathbf{Z}_s-\tilde{\mathbf{Z}}_s, && \beta_{z,s}=\tilde{\mathbf{Z}}_s-\mathbf{z}_s\ \ (s=e,p,T), && \bar{\alpha}_{z,s}=\bar{\mathbf{Z}}_s-\tilde{\tilde{\mathbf{Z}}}_s, && \bar{\beta}_{z,s}=\tilde{\tilde{\mathbf{Z}}}_s-\bar{\mathbf{z}}_s\ \ (s=e,p).
\end{aligned}$$

Suppose that (1.1a)-(1.5) satisfies positive condition (C), and the exact solutions satisfy regularity (R). From the theory of Weiser and Wheeler [21] and the discussions of Arbogast, Wheeler and Yotov [2,31], it is easy to see that the auxiliary functions $\{\tilde{\Psi},\tilde{\mathbf{U}},\tilde{S},\tilde{\mathbf{Z}}_s,\tilde{\tilde{\mathbf{Z}}}_s,(s=e,p),\tilde{H},\tilde{Z}_H\}$ of (5.1) and (5.4) exist and are unique.

Lemma 5.1. *The coefficients and exact solutions of* (1.1a)-(1.5) *are supposed to satisfy* (C) *and* (R)*, then there exist two positive constants* $\bar{C}_1,\bar{C}_2>0$ *independent of* h *and* Δt *such that*

$$\begin{aligned}
&||\eta||_{\bar{m}}+\sum_{s=e,p,T}||\zeta_s||_{\bar{m}}+|||\boldsymbol{\rho}_T|||+\sum_{s=e,p,T}|||\boldsymbol{\beta}_{z,s}|||\\
&\quad+\sum_{s=e,p}|||\bar{\boldsymbol{\beta}}_{z,s}|||+\left|\left|\frac{\partial\eta}{\partial t}\right|\right|_{\bar{m}}+\sum_{s=e,p,T}\left|\left|\frac{\partial\zeta_s}{\partial t}\right|\right|_{\bar{m}}\le\bar{C}_1\{h_\psi^2+h_s^2\},
\end{aligned}\tag{5.5a}$$

$$|||\tilde{\mathbf{U}}|||_\infty+\sum_{s=e,p,T}|||\tilde{\mathbf{Z}}_s|||_\infty+\sum_{s=e,p}|||\tilde{\tilde{\mathbf{Z}}}_s|||_\infty\le\bar{C}_2. \tag{5.5b}$$

We estimate π and σ first. By subtracting (5.1a) ($t=t_m$) and (5.1b) ($t=t_m$), respectively, from (3.3a) and (3.3b), we have

$$\big(D_x\sigma_m^x+D_y\sigma_m^y+D_z\sigma_m^z,v\big)_{\bar{m}}=\alpha\big(E_m-e_m-P_m+p_m,v\big)_{\bar{m}},\qquad \forall v\in S_h, \tag{5.6a}$$

$$(\sigma_m^x,w^x)_x+\big(\sigma_m^y,w^y\big)_y+(\sigma_m^z,w^z)_z-\big(\pi_m,D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}}=0,\qquad \forall \mathbf{w}\in V_h. \tag{5.6b}$$

Taking $v=\pi_m$ in (5.6a) and $\mathbf{w}=\sigma_m$ in (5.6b), we have the combination equation

$$(\sigma_m^x,\sigma_m^x)_x+\big(\sigma_m^y,\sigma_m^y\big)_y+(\sigma_m^z,\sigma_m^z)_z=\alpha\big(E_m-e_m-P_m+p_m,\pi_m\big)_{\bar{m}}. \tag{5.7}$$

Applying Lemmas 2.1, 2.2, 2.3 and 5.1, we have

$$|||\sigma_m|||^2=\alpha\big(E_m-e_m-P_m+p_m,\pi_m\big)_{\bar{m}}. \tag{5.8}$$

A duality method is introduced to address $\pi_m\in S_h$ [33,34]. Consider the following elliptic problem,

$$\nabla\cdot\omega=\pi_m,\qquad X=(x,y,z)^T\in\Omega, \tag{5.9a}$$

$$\omega=\nabla\psi,\qquad X\in\Omega, \tag{5.9b}$$

$$\omega\cdot\gamma=0,\qquad X\in\partial\Omega. \tag{5.9c}$$

It follows from the regularity of (5.9) that

$$\sum_{s=x,y,z}\Big|\Big|\frac{\partial\omega^s}{\partial s}\Big|\Big|_{\bar{m}}^2\le K||\pi_m||_{\bar{m}}^2. \tag{5.10}$$

Let $\tilde{\omega}\in V_h$ be defined by

$$\Big(\frac{\partial\tilde{\omega}^s}{\partial s},v\Big)_{\bar{m}}=\Big(\frac{\partial\omega^s}{\partial s},v\Big)_{\bar{m}},\quad \forall v\in S_h,\quad s=x,y,z. \tag{5.11a}$$

The solution $\tilde{\omega}$ exists and satisfies

$$\sum_{s=x,y,z}\Big|\Big|\frac{\partial\tilde{\omega}^s}{\partial s}\Big|\Big|_{\bar{m}}^2\le\sum_{s=x,y,z}\Big|\Big|\frac{\partial\omega^s}{\partial s}\Big|\Big|_{\bar{m}}^2. \tag{5.11b}$$

By Lemma 2.3, (5.9), (5.10) and (5.8), we obtain

$$\begin{aligned}||\pi_m||_{\bar{m}}^2&=(\pi_m,\nabla\cdot\omega)_{\bar{m}}=\big(\pi_m,D_x\tilde{\omega}^x+D_y\tilde{\omega}^y+D_z\tilde{\omega}^z\big)_{\bar{m}}\\&=\sum_{s=x,y,z}(\sigma_m^s,\tilde{\omega}^s)_s\le K|||\tilde{\omega}|||\cdot|||\sigma_m|||.\end{aligned} \tag{5.12}$$

Similarly, we have

$$
\begin{aligned}
|||\tilde{\omega}|||^2 \leq & \sum_{s=x,y,z} ||D_s\tilde{\omega}^s||_{\bar{m}}^2 = \sum_{s=x,y,z} \left|\left|\frac{\partial\tilde{\omega}^s}{\partial s}\right|\right|_{\bar{m}}^2 \\
\leq & \sum_{s=x,y,z} \left|\left|\frac{\partial\omega^s}{\partial s}\right|\right|_{\bar{m}}^2 \leq K||\pi_m||_{\bar{m}}^2.
\end{aligned} \tag{5.13}
$$

Substituting (5.13) into (5.12) and addressing (5.8), we obtain

$$
||\pi_m||_{\bar{m}}^2 + |||\sigma_m|||^2 \leq K\Big\{||\xi_{e,m}||_{\bar{m}}^2 + ||\xi_{p,m}||_{\bar{m}}^2 + h_\psi^4 + h_s^4\Big\}. \tag{5.14}
$$

The electron concentration equation (1.1b) is estimated. At $t=t^n$, error equations are formulated as follows

$$
\begin{aligned}
&\left(\phi\frac{e^n-e^{n-1}}{\Delta t_s},v\right)_{\bar{m}} - \frac{2}{3}\big(\nabla\cdot\mathbf{g}_e^n,v\big)_{\bar{m}} + \frac{2}{3}\big(\nabla\cdot\mathbf{z}_e^n,v\big)_{\bar{m}} \\
&=\frac{1}{\Delta t_s}\left(\frac{1}{3}\delta e^{n-1},v\right)_{\bar{m}} - \frac{2}{3}\big(R_1(e^n,p^n,T^n),v\big)_{\bar{m}} - \big(\rho^n,v\big)_{\bar{m}}, \qquad \forall v\in S_h, &\text{(5.15a)}\\
&\big(\bar{z}_e^{x,n},w^x\big)_x + \big(\bar{z}_e^{y,n},w^y\big)_y + \big(\bar{z}_e^{z,n},w^z\big)_z = \left(e^n,\sum_{s=x,y,z} D_s w^s\right)_{\bar{m}}, \qquad \forall \mathbf{w}\in V_h, &\text{(5.15b)}\\
&\big(z_e^{x,n},w^x\big)_x + \big(z_e^{y,n},w^y\big)_y + \big(z_e^{z,n},w^z\big)_z = \sum_{s=x,y,z}\big(D_e\bar{z}_e^{s,n},w^s\big)_s, \qquad \forall \mathbf{w}\in V_h, &\text{(5.15c)}
\end{aligned}
$$

where

$$
\rho^n = \frac{2}{3}\frac{\partial e^n}{\partial t} - \phi\frac{1}{\Delta t_s}\left(e^n - \frac{4}{3}e^{n-1} + \frac{1}{3}e^{n-2}\right).
$$

Subtracting (3.7) from (5.15) and using the L^2-projection (5.2), we have

$$
\begin{aligned}
&\left(\frac{\xi_e^n-\xi_e^{n-1}}{\Delta t_s},v\right)_{\bar{m}} - \frac{2}{3}\big(\nabla\cdot(\mathbf{G}_e^n-\mathbf{g}_e^n),v\big)_{\bar{m}} + \frac{2}{3}\left(\sum_{s=x,y,z} D_s\alpha_{z,e}^{s,n},v\right)_{\bar{m}} \\
&=\frac{1}{\Delta t_s}\left(\frac{1}{3}\delta\xi_e^{n-1},v\right)_{\bar{m}} + \big(\rho^n,v\big)_{\bar{m}} - \frac{2}{3}\big(R_1(e^n,p^n,T^n) - R_1(\hat{E}(2)(E,P,H)^n),v\big)_{\bar{m}}, \quad \forall v\in S_h, &\text{(5.16a)}\\
&\big(\bar{\alpha}_{z,e}^{x,n},w^x\big)_x + \big(\bar{\alpha}_{z,e}^{y,n},w^y\big)_y + \big(\bar{\alpha}_{z,e}^{z,n},w^z\big)_z = \left(\xi_e^n,\sum_{s=x,y,z} D_s w^s\right)_{\bar{m}}, \qquad \mathbf{w}\in V_h, &\text{(5.16b)}\\
&\big(\alpha_{z,e}^{x,n},w^x\big)_x + \big(\alpha_{z,e}^{y,n},w^y\big)_y + \big(\alpha_{z,e}^{z,n},w^z\big)_z = \sum_{s=x,y,z}\big(D_e\bar{\alpha}_{z,e}^{s,n},w^s\big)_s, \qquad \mathbf{w}\in V_h. &\text{(5.16c)}
\end{aligned}
$$

Taking $v=\xi_e^n$ in (5.16a), $\mathbf{w}=\alpha_{z,e}^n$ in (5.16b), and $\mathbf{w}=\bar{\alpha}_{z,e}^n$ in (5.16c), multiplying both sides of (5.16b) and (5.16c) by $\frac{2}{3}$, then subtracting (5.16c) from the sum of (5.16a) and (5.16b), we obtain

$$
\begin{aligned}
&\left(\frac{\xi_e^n-\xi_e^{n-1}}{\Delta t_s},\xi_e^n\right)_{\bar{m}}+\frac{2}{3}\sum_{s=x,y,z}\left(D_e\bar{\alpha}_{z,e}^{s,n},\bar{\alpha}_{z,e}^{s,n}\right)_s\\
=&\frac{2}{3}\left(\nabla\cdot(\mathbf{G}_e^n-\mathbf{g}_e^n),\xi_e^n\right)_{\bar{m}}+\frac{1}{3\Delta t_s}\left(\delta\xi_e^{n-1},\xi_e^n\right)_{\bar{m}}+\left(\rho^n,\xi_e^n\right)_{\bar{m}}-\left(\frac{\zeta_e^n-\zeta_e^{n-1}}{\Delta t_s},\xi_e^n\right)_{\bar{m}}\\
&-\frac{2}{3}\left(R_1(e^n,p^n,T^n)-R_1(\check{E}(2)(E,P,H)^n),\xi_e^n\right)_{\bar{m}}\\
=&T_1+T_2+T_3+T_4+T_5. \qquad (5.17)
\end{aligned}
$$

The terms on the left-hand side of (5.17) are estimated as follows,

$$
\left(\frac{\xi_e^n-\xi_e^{n-1}}{\Delta t_s},\xi_e^n\right)_{\bar{m}}=\frac{1}{2\Delta t_s}\left\{||\xi_e^n||_{\bar{m}}^2-||\xi_e^{n-1}||_{\bar{m}}^2\right\}+\frac{1}{2\Delta t_s}||\xi_e^n-\xi_e^{n-1}||_{\bar{m}}^2, \qquad (5.18a)
$$

$$
\frac{2}{3}\sum_{s=x,y,z}\left(D_e\bar{\alpha}_{z,e}^{s,n},\bar{\alpha}_{z,e}^{s,n}\right)_s\geq\frac{2}{3}D_*|||\bar{\alpha}_{z,e}^n|||^2. \qquad (5.18b)
$$

The terms on the right-hand side are estimated one by one.

$$
T_1=\frac{2}{3}\left(\nabla\cdot(\mathbf{G}_e^n-\mathbf{g}_e^n),\xi_e^n\right)_{\bar{m}}=-\frac{2}{3}\left(\mathbf{G}_e^n-\mathbf{g}_e^n,\nabla\xi_e^n\right)_{\bar{m}}\leq\varepsilon|||\bar{\alpha}_{z,e}^n|||^2+K||\mathbf{G}_e^n-\mathbf{g}_e^n||_{\bar{m}}^2. \qquad (5.19a)
$$

With σ being the shared plane, γ_r being the unit normal vector and X_l being the barycentre, then,

$$
\int_\sigma \mathbf{g}_e^n\cdot\gamma_r=\int_\omega \mu_e e^n(\mathbf{u}^n\cdot\gamma_r)ds. \qquad (5.19b)
$$

By the regularity (R) and the mean value theorem for integrals,

$$
\frac{1}{\mathrm{mes}(\sigma)}\int_\sigma \mathbf{g}_e^n\cdot\gamma_r-(\mu_e(\mathbf{u}^n\cdot\gamma_r)e^n)(X_l)=\mathcal{O}(h_s). \qquad (5.19c)
$$

Therefore,

$$
\begin{aligned}
&\frac{1}{\mathrm{mes}(\sigma)}\int_\sigma(\mathbf{G}_e^n-\mathbf{g}_e^n)\cdot\gamma_r\\
=&E_\sigma^n(\mu_e\bar{E}\mathbf{U}^n\cdot\gamma_r)(X_l)-(\mu_e(\mathbf{u}^n\cdot\gamma_r)e^n)(X_l)+\mathcal{O}(h_s)\\
=&\left(E_\sigma^n-e^n(X_l)\right)\left(\mu_e\bar{E}\mathbf{U}^n\cdot\gamma_r\right)(X_l)+e^n(X_l)\left(\mu_e(\bar{E}\mathbf{U}^n-\mathbf{u}^n)\cdot\gamma_r\right)(X_l)+\mathcal{O}(h_s). \qquad (5.19d)
\end{aligned}
$$

From the regularity of e^n, Lemma 5.1 and the discussion in [21,31,32], we have

$$
|E_\sigma^n-e^n(X_l)|\leq|\xi_e^n|+\mathcal{O}(h_s), \qquad (5.19e)
$$

$$
|\bar{E}\mathbf{U}^n-\mathbf{u}^n|\leq K\{|\xi_{e,m-1}|+|\xi_{e,m-2}|\}+\mathcal{O}(h_s)+\mathcal{O}(\Delta t_\psi^2). \qquad (5.19f)
$$

Using (5.19ab)-(5.19af), we obtain

$$||\mathbf{G}_e^n-\mathbf{g}_e^n||_{\bar{m}}^2\le K\Big\{||\xi_e^n||_{\bar{m}}^2+||\xi_{e,m-1}||_{\bar{m}}^2+||\xi_{e,m-2}||_{\bar{m}}^2+h_s^2+(\Delta t_\psi)^4\Big\}. \tag{5.20}$$

Thus, we get the estimate of T_1,

$$\begin{aligned}T_1=&\frac{2}{3}\big(\nabla\cdot(\mathbf{G}_e^n-\mathbf{g}_e^n),\xi_e^n\big)_{\bar{m}}\\ \le&\varepsilon|||\bar{\alpha}_{z,e}^n|||^2+K\Big\{||\xi_e^n||_{\bar{m}}^2+||\xi_{e,m-1}||_{\bar{m}}^2+||\xi_{e,m-2}||_{\bar{m}}^2+h_s^2+(\Delta t_\psi)^4\Big\}.\end{aligned} \tag{5.21a}$$

The other terms of (5.17) are estimated as follows,

$$\begin{aligned}T_2=&\frac{1}{3\Delta t_s}\big(\xi_e^{n-1}-\xi_e^{n-2},\xi_e^n\big)_{\bar{m}}=\frac{1}{3\Delta t_s}\big(\xi_e^{n-1}-\xi_e^{n-2},\xi_e^n-\xi_e^{n-1}+\xi_e^{n-1}\big)_{\bar{m}}\\ \le&\frac{1}{3\Delta t_s}\Big\{\frac{1}{2}||\xi_e^{n-1}-\xi_e^{n-2}||_{\bar{m}}^2+\frac{1}{2}||\xi_e^n-\xi_e^{n-1}||_{\bar{m}}^2+\frac{1}{2}||\xi_e^{n-1}-\xi_e^{n-2}||_{\bar{m}}^2\\ &+\frac{1}{2}\big[||\xi_e^{n-1}||_{\bar{m}}^2-||\xi_e^{n-2}||_{\bar{m}}^2\big]\Big\}\\ =&\frac{1}{3\Delta t_s}\Big\{||\xi_e^{n-1}-\xi_e^{n-2}||_{\bar{m}}^2+\frac{1}{2}||\xi_e^n-\xi_e^{n-1}||_{\bar{m}}^2+\frac{1}{2}\big[||\xi_e^{n-1}||_{\bar{m}}^2-||\xi_e^{n-2}||_{\bar{m}}^2\big]\Big\},\end{aligned} \tag{5.21b}$$

$$T_3\le K(\Delta t_s)^4||\frac{\partial^3 e}{\partial t^3}||_{\bar{m}}^2+K||\xi_e^{n-1}||_{\bar{m}}^2, \tag{5.21c}$$

$$T_4\le K\Big\{||\xi_e^n||_{\bar{m}}^2+h_s^4\Big\}, \tag{5.21d}$$

$$T_5\le K\Big\{||\xi_e^n||_{\bar{m}}^2+||\xi_e^{n-1}||_{\bar{m}}^2+||\xi_p^{n-1}||_{\bar{m}}^2+||\xi_T^{n-1}||_{\bar{m}}^2+(\Delta t_s)^4+h_s^4\Big\}. \tag{5.21e}$$

Substituting (5.18)-(5.21a) into (5.17), we have

$$\begin{aligned}&\frac{1}{2\Delta t_s}\Big\{||\xi_e^n||_{\bar{m}}^2-||\xi_e^{n-1}||_{\bar{m}}^2\Big\}+\frac{1}{2\Delta t_s}||\xi_e^n-\xi_e^{n-1}||_{\bar{m}}^2+\frac{1}{2}D_*|||\bar{\alpha}_{z,e}^n|||^2\\ \le&\frac{1}{3\Delta t_s}\Big\{||\xi_e^{n-1}-\xi_e^{n-2}||_{\bar{m}}^2+\frac{1}{2}||\xi_e^n-\xi_e^{n-1}||_{\bar{m}}^2+\frac{1}{2}\big[||\xi_e^{n-1}||_{\bar{m}}^2-||\xi_e^{n-2}||_{\bar{m}}^2\big]\Big\}\\ &+K\Big\{(\Delta t_s)^3\Big|\Big|\frac{\partial^3 e}{\partial t^3}\Big|\Big|_{\bar{L}^2(t^{n-2},t^n,\bar{m})}^2+(\Delta t_\psi)^3\Big|\Big|\frac{\partial^2\mathbf{u}}{\partial t^2}\Big|\Big|_{\bar{L}^2(t_{m-2},t_{m-1},\bar{m})}^2\Big\}\\ &+K\Big\{||\xi_e^n||_{\bar{m}}^2+||\xi_e^{n-1}||_{\bar{m}}^2+||\xi_p^{n-1}||_{\bar{m}}^2+||\xi_T^{n-1}||_{\bar{m}}^2+||\xi_{e,m-1}||_{\bar{m}}^2\\ &+||\xi_{e,m-2}||_{\bar{m}}^2+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}.\end{aligned} \tag{5.22}$$

Furthermore,

$$\begin{aligned}&\frac{1}{2\Delta t_s}\Big\{||\xi_e^n||_{\bar{m}}^2-||\xi_e^{n-1}||_{\bar{m}}^2\Big\}+\frac{1}{3\Delta t_s}\Big\{||\xi_e^n-\xi_e^{n-1}||_{\bar{m}}^2-||\xi_e^{n-1}-\xi_e^{n-2}||_{\bar{m}}^2\Big\}+\frac{1}{2}D_*|||\bar{\alpha}_{z,e}^n|||^2\\ \le&\frac{1}{6\Delta t_s}\Big\{||\xi_e^{n-1}||_{\bar{m}}^2-||\xi_e^{n-2}||_{\bar{m}}^2\Big\}+K\Big\{(\Delta t_s)^3\Big|\Big|\frac{\partial^3 e}{\partial t^3}\Big|\Big|_{\bar{L}^2(t^{n-2},t^n,\bar{m})}^2+(\Delta t_\psi)^3\Big|\Big|\frac{\partial^2\mathbf{u}}{\partial t^2}\Big|\Big|_{\bar{L}^2(t_{m-2},t_{m-1},\bar{m})}^2\Big\}\end{aligned}$$

$$+K\Big\{||\xi_e^n||_{\bar m}^2+||\xi_e^{n-1}||_{\bar m}^2+||\xi_p^{n-1}||_{\bar m}^2+||\xi_T^{n-1}||_{\bar m}^2+||\xi_{e,m-1}||_{\bar m}^2$$
$$+||\xi_{e,m-2}||_{\bar m}^2+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}. \tag{5.23}$$

Multiplying both sides of (5.23) by Δt_s and making the sum on n, we obtain

$$\begin{aligned}
&\frac{1}{2}\Big\{||\xi_e^N||_{\bar m}^2-||\xi_e^1||_{\bar m}^2\Big\}+\frac{1}{3}\Big\{||\xi_e^N-\xi_e^{N-1}||_{\bar m}^2-||\xi_e^1-\xi_e^0||_{\bar m}^2\Big\}+\frac{1}{2}D_*\sum_{n=1}^N|||\bar\alpha_{z,e}^n|||^2\Delta t_s\\
\le&\frac{1}{6}\Big\{||\xi_e^{N-1}||_{\bar m}^2-||\xi_e^0||_{\bar m}^2\Big\}+K\Big\{(\Delta t_{\psi,1})^3+(\Delta t_\psi)^4+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}\\
&+K\sum_{n=1}^N\Big\{||\xi_e^n||_{\bar m}^2+||\xi_p^n||_{\bar m}^2+||\xi_T^n||_{\bar m}^2\Big\}\Delta t_s\\
\le&\frac{1}{6}\Big\{||\xi_e^N-\xi_e^{N-1}||_{\bar m}^2+||\xi_e^N||_{\bar m}^2-||\xi_e^0||_{\bar m}^2\Big\}+K\Big\{(\Delta t_{\psi,1})^3+(\Delta t_\psi)^4+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}\\
&+K\sum_{n=1}^N\Big\{||\xi_e^n||_{\bar m}^2+||\xi_p^n||_{\bar m}^2+||\xi_T^n||_{\bar m}^2\Big\}\Delta t_s.
\end{aligned} \tag{5.24}$$

Error estimate of the electron concentration is given by

$$\begin{aligned}
&\frac{1}{3}||\xi_e^N||_{\bar m}^2+\frac{1}{6}||\xi_e^N-\xi_e^{N-1}||_{\bar m}^2+\frac{1}{2}D_*\sum_{n=1}^N|||\bar\alpha_{z,e}^n|||^2\Delta t_s\\
\le&\frac{1}{6}\Big\{3||\xi_e^1||_{\bar m}^2-||\xi_e^0||_{\bar m}^2\Big\}+\frac{1}{3}\Big\{||\xi_e^1-\xi_e^0||_{\bar m}^2+K\Big\{(\Delta t_{\psi,1})^3+(\Delta t_\psi)^4+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}\\
&+K\sum_{n=1}^N\Big\{||\xi_e^n||_{\bar m}^2+||\xi_p^n||_{\bar m}^2+||\xi_T^n||_{\bar m}^2\Big\}\Delta t_s.
\end{aligned} \tag{5.25}$$

Similarly, the hole concentration (1.1c) is estimated as follow

$$\begin{aligned}
&\frac{1}{3}||\xi_p^N||_{\bar m}^2+\frac{1}{6}||\xi_p^N-\xi_p^{N-1}||_{\bar m}^2+\frac{1}{2}D_*\sum_{n=1}^N|||\bar\alpha_{z,p}^n|||^2\Delta t_s\\
\le&\frac{1}{6}\Big\{3||\xi_p^1||_{\bar m}^2-||\xi_p^0||_{\bar m}^2\Big\}+\frac{1}{3}\Big\{||\xi_p^1-\xi_p^0||_{\bar m}^2+K\Big\{(\Delta t_{\psi,1})^3+(\Delta t_\psi)^4+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}\\
&+K\sum_{n=1}^N\Big\{||\xi_e^n||_{\bar m}^2+||\xi_p^n||_{\bar m}^2+||\xi_T^n||_{\bar m}^2\Big\}\Delta t_s.
\end{aligned} \tag{5.26}$$

Finally, the heat conduction equation (1.1d) is argued. Subtracting (5.4a) $(t=t^n)$ and (5.4b) $(t=t^n)$ from (3.12a) and (3.12b), respectively, we obtain

$$\begin{aligned}
&\left(\rho\frac{\xi_T^n-\xi_T^{n-1}}{\Delta t_s},v\right)_{\bar m}+\frac{2}{3}\sum_{s=x,y,z}\left(D_s\bar\alpha_{z,T}^{s,n},v\right)_s\\
=&\frac{1}{\Delta t_s}\left(\frac{1}{3}\delta\xi_T^{n-1},v\right)_{\bar m}+\left(r^n,v\right)_{\bar m}+\frac{2}{3}\Big(\big[(\mathbf{Z}_p^{n-1}+\mu_pP^{n-1}\bar E\mathbf{U}^n)-(\mathbf{Z}_e^{n-1}+\mu_eE^{n-1}\bar E\mathbf{U}^n)\big]\cdot\bar E\mathbf{U}^n
\end{aligned}$$

$$-\big[(\mathbf{z}_p^n+\mu_p p^n\mathbf{u}^n)-(\mathbf{z}_e^n+\mu_e e^n\mathbf{u}^n)\big]\cdot\mathbf{u}^n,v\Big)_{\bar{m}}, \qquad \forall v\in S_h, \tag{5.27a}$$

$$\big(\alpha_{z,T}^{x,n},w^x\big)_x+\big(\alpha_{z,T}^{y,n},w^y\big)_y+\big(\alpha_{z,T}^{z,n},w^z\big)_z=\Big(\xi_T^n,\sum_{s=x,y,z}D_sw^s\Big)_{\bar{m}}, \qquad \forall \mathbf{w}\in V_h, \tag{5.27b}$$

where

$$r^n=\frac{2}{3}\rho\frac{\partial T^n}{\partial t}-\frac{\rho}{\Delta t_s}\Big(T^n-\frac{4}{3}T^{n-1}+\frac{1}{3}T^{n-2}\Big).$$

An induction hypothesis is introduced

$$\max_{0\le m\le M}|||\sigma_m|||_\infty\le 1, \quad (\Delta t,h)\to 0, \tag{5.28}$$

and the partition parameters are supposed to satisfy

$$\big(\Delta t_{\psi,1}\big)^{\frac{3}{2}}+\big(\Delta t_\psi\big)^2+\big(\Delta t_s\big)^2=o\big(h_\psi^{\frac{3}{2}}\big), \qquad (\Delta t,h)\to 0, \tag{5.29a}$$

$$h_s=o\big(h_\psi^{\frac{3}{2}}\big), \qquad (\Delta t,h)\to 0. \tag{5.29b}$$

Taking $v=\xi_T^n$ in (5.27a), multiplying both sides of (5.27b) by $\frac{2}{3}$ and taking $\mathbf{w}=\alpha_{z,T}^n$, and summing (5.27a) and (5.27b), we have

$$\begin{aligned}
&\Big(\rho\frac{\xi_T^n-\xi_T^{n-1}}{\Delta t_s},\xi_T^n\Big)_{\bar{m}}+|||\sigma_m|||^2\\
=&\frac{1}{\Delta t_s}\Big(\frac{1}{3}\delta\xi_T^{n-1},\xi_T^n\Big)_{\bar{m}}+\big(r^n,\xi_T^n\big)_{\bar{m}}+\frac{2}{3}\Big(\big[(\mathbf{Z}_p^{n-1}+\mu_pP^{n-1}\bar{E}\mathbf{U}^n)\\
&-(\mathbf{Z}_e^{n-1}+\mu_eE^{n-1}\bar{E}\mathbf{U}^n)\big]\cdot\bar{E}\mathbf{U}^n-\big[(\mathbf{z}_p^n+\mu_pp^n\mathbf{u}^n)-(\mathbf{z}_e^n+\mu_ee^n\mathbf{u}^n)\big]\cdot\mathbf{u}^n,\xi_T^n\Big)_{\bar{m}}.
\end{aligned} \tag{5.30}$$

By estimating both sides of (5.30) and using (5.28), we get

$$\begin{aligned}
&\frac{1}{3}||\rho^{\frac{1}{2}}\xi_T^N||_{\bar{m}}^2+\frac{1}{6}||\rho^{\frac{1}{2}}(\xi_T^N-\xi_T^{N-1})||_{\bar{m}}^2+\sum_{n=1}^N|||\alpha_{z,T}^n|||^2\Delta t_s\\
\le&\frac{1}{6}\Big\{3||\rho^{\frac{1}{2}}\xi_T^1||_{\bar{m}}^2-||\rho^{\frac{1}{2}}\xi_T^0||_{\bar{m}}^2\Big\}+\frac{1}{3}\Big\{||\rho^{\frac{1}{2}}(\xi_T^1-\xi_T^0)||_{\bar{m}}^2+\varepsilon\sum_{n=1}^N\Big\{|||\bar{\alpha}_{z,e}^n|||^2+|||\bar{\alpha}_{z,p}^n|||^2\Big\}\Delta t_s\\
&+K\Big\{(\Delta t_{\psi,1})^3+(\Delta t_\psi)^4+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}\\
&+\sum_{n=1}^N\Big\{||\xi_e^n||_{\bar{m}}^2+||\xi_p^n||_{\bar{m}}^2+||\rho^{\frac{1}{2}}\xi_T^n||_{\bar{m}}^2\Big\}\Delta t_s.
\end{aligned} \tag{5.31}$$

Considering (5.25), (5.26) and (5.31) together, we have

$$\begin{aligned}
&\frac{1}{3}\Big\{\sum_{s=e,p}||\xi_s^N||_{\bar{m}}^2+||\rho^{\frac{1}{2}}\xi_T^N||_{\bar{m}}^2\Big\}+\frac{1}{6}\Big\{\sum_{s=e,p}||\xi_s^N-\xi_s^{N-1}||_{\bar{m}}^2+||\rho^{\frac{1}{2}}(\xi_T^N-\xi_T^{N-1})||_{\bar{m}}^2\Big\}\\
&\quad+\frac{1}{4}D_*\sum_{n=1}^N\sum_{s=e,p}|||\alpha_{z,s}^n|||^2\Delta t_s+\sum_{n=1}^N|||\alpha_{z,T}^n|||^2\Delta t_s\\
&\le\frac{1}{6}\Big\{\sum_{s=e,p}[3||\xi_s^1||_{\bar{m}}^2-||\xi_s^0||_{\bar{m}}^2]+3||\rho^{\frac{1}{2}}\xi_T^1||_{\bar{m}}^2-||\rho^{\frac{1}{2}}\xi_T^0||_{\bar{m}}^2\Big\}\\
&\quad+\frac{1}{3}\Big\{\sum_{s=e,p}||\xi_s^1-\xi_s^0||_{\bar{m}}^2+||\rho^{\frac{1}{2}}(\xi_T^1-\xi_T^0)||_{\bar{m}}^2\Big\}+K\Big\{(\Delta t_{\psi,1})^3+(\Delta t_\psi)^4+(\Delta t_s)^4+h_\psi^4+h_s^2\Big\}\\
&\quad+K\sum_{n=1}^N\Big\{||\xi_e^n||_{\bar{m}}^2+||\xi_p^n||_{\bar{m}}^2+||\rho^{\frac{1}{2}}\xi_T^n||_{\bar{m}}^2\Big\}\Delta t_s. \qquad (5.32)
\end{aligned}$$

Applying the discrete Gronwall Lemma and using initial approximations we have

$$\begin{aligned}
&\sum_{s=e,p,T}||\xi_s^N||_{\bar{m}}^2+\sum_{n=1}^N\Big\{\sum_{s=e,p}|||\bar{\alpha}_{z,s}^n|||^2+|||\alpha_{z,T}^n|||^2\Big\}\Delta t_s\\
&\le K\Big\{h_s^2+h_\psi^4+(\Delta t_s)^4+\big(\Delta t_{\psi,1}\big)^3+\big(\Delta t_\psi\big)^4\Big\}. \qquad (5.33)
\end{aligned}$$

It follows from (5.33) and (5.14),

$$\sup_{0\le n\le N}\Big\{||\pi_m||_{\bar{m}}^2+|||\sigma_m|||^2\Big\}\le K\Big\{h_s^2+h_\psi^4+(\Delta t_s)^4+\big(\Delta t_{\psi,1}\big)^3+\big(\Delta t_\psi\big)^4\Big\}. \qquad (5.34)$$

It remains to verify the induction hypothesis (5.28). Using (5.34) and (5.29), we can prove (5.28) easily. The following theorem is derived by using (5.32), (5.33) and Lemma 5.1.

Theorem 5.1. *Suppose that exact solutions of* (1.1a)-(1.5) *are regular* (R)*, and the coefficients are positive definite* (C)*. Numerical solutions are obtained by using the scheme of* (3.3), (3.7), (3.10) *and* (3.12)*. The partition is supposed to satisfy* (5.29)*. Then,*

$$\begin{aligned}
&||\psi-\Psi||_{\bar{L}^\infty(J;\bar{m})}+||\mathbf{u}-\mathbf{U}||_{\bar{L}^\infty(J;V)}+\sum_{s=e,p}||s-S||_{\bar{L}^\infty(J;\bar{m})}\\
&\quad+||T-H||_{\bar{L}^\infty(J;\bar{m})}+\sum_{s=e,p}||\bar{\mathbf{z}}_s-\bar{\mathbf{Z}}_s||_{\bar{L}^2(J;V)}+||\mathbf{z}_T-\mathbf{Z}_T||_{\bar{L}^2(J;V)}\\
&\le M^*\Big\{h_\psi^2+h_s+(\Delta t_s)^2+(\Delta t_{\psi,1})^{\frac{3}{2}}+(\Delta t_\psi)^2\Big\}, \qquad (5.35)
\end{aligned}$$

where

$$||g||_{\bar{L}^\infty(J;X)}=\sup_{n\Delta t\le T}||g^n||_X,\quad ||g||_{\bar{L}^2(J;X)}=\sup_{L\Delta t\le T}\Big\{\sum_{n=0}^L||g^n||_X^2\Delta t_c\Big\}^{\frac{1}{2}},$$

and the constant M^* is dependent on ψ, $\mathbf{u}$, e, p and T and their derivatives.

6 Numerical experiment

In this section, a nonstationary convection-dominated diffusion problem is discussed to support theoretical analysis. The mathematical model is formulated by

$$\begin{cases} \dfrac{\partial u}{\partial t}+\nabla\cdot(-a(x)\nabla u+\mathbf{b}u)=f, & (x,y,z)\in\Omega, \quad t\in(0,T], \\ u|_{t=0}=x(1-x)y(1-y)z(1-z), & (x,y,z)\in\Omega, \\ u|_{\partial\Omega}=0, & t\in(0,T]. \end{cases} \tag{6.1}$$

Problem I (P-I, convection-dominated case).

$$a(x)=0.01, \quad b_1=(1+x\cos\alpha)\cos\alpha, \quad b_2=(1+y\sin\alpha)\sin\alpha, \quad b_3=1, \quad \alpha=\frac{\pi}{12}.$$

Problem II (P-II, strongly convection-dominated case).

$$a(x)=10^{-5}, \quad b_1=1, \quad b_2=1, \quad b_3=-2.$$

Take $\Omega=(0,1)\times(0,1)\times(0,1)$, $t\in[0,\frac{1}{2}]$ and $\Delta t=\frac{1}{12}$. f is chosen to obtain the exact solution

$$u=e^{t/4}x(1-x)y(1-y)z(1-z).$$

U denotes the numerical solution. Numerical data are illustrated in Tables 2-4.

Let $||\cdot||$ denote the discrete l^2 norm. N denotes the number of elements in a direction. The upwind-block-centered finite difference method and the finite difference method are denoted by UBCFDM and FDM, respectively. Numerical data are illustrated for P-I and P-II in Tables 2 and 3. We conclude that FDM can solve the convection-dominated problem but becomes invalid for strongly convection-dominated problems. FDM has oscillation and dispersion when the step is small. UBCFDM can solve both convection-dominated diffusion equation and strongly convection-dominated case well because it can avoid numerical oscillation. So UBCFDM is better in solving convection-dominated problems than the finite element method and FDM.

Table 2: Numerical data of $||u-U||$ for P-I.

N	8	16	24
UBCFDM	$5.7604e-7$	$7.4580e-8$	$3.9599e-8$
FDM	$1.2686e-6$	$3.4144e-7$	$1.5720e-7$

Table 3: Numerical data $||u-U||$ for P-II.

N	8	16	24
UBCFDM	$5.1822e-7$	$1.0127e-7$	$6.8874e-8$
FDM	$3.3386e-5$	$3.2242e+9$	overflow

Table 4: Comparison of two schemes (M,S).

N	8	16	24
M	$2.8160e-7$	$6.5832e-8$	$7.9215e-8$
S	$5.7604e-7$	$7.4580e-8$	$3.9599e-8$

Table 5: Numerical data for positive semi-definite problems.

N	8	16	24
P-III	$8.0682e-7$	$5.5915e-8$	$1.2303e-8$
P-IV	$1.6367e-5$	$2.4944e-6$	$4.2888e-7$

The single step method and multistep method are compared. The convection-dominated diffusion equation (P-I) is solved by the upwind-block-centered multistep scheme (M) and upwind-block-centered single-step scheme (S), respectively. The former adopts $\Delta t=\frac{T}{3}$ and the latter adopts $\Delta t=\frac{T}{6}$. From Table 4, we conclude that the multistep method has the advantages of single step scheme and improves the accuracy with small-scaled computational work.

Furthermore, two positive semi-definite problems are considered to show the efficiency and application.

P-III:

$$a(x)=x(1-x),\quad b_1=1,\quad b_2=1,\quad b_3=0.$$

P-IV:

$$a(x)=\Big(x-\frac{1}{2}\Big)^2,\quad b_1=-3,\quad b_2=1,\quad b_3=0.$$

Numerical data are obtained by using the upwind-block-centered scheme in Table 5 for two positive semi-definite problems, P-III and P-IV. We find that the numerical results are satisfactory for the problem with positive semi-definite diffusion matrix.

7 Conclusions and discussions

Numerical simulation of the three dimensional semiconductor device transient behavior problem of heat conduction is discussed in this paper. An upwind-block-centered multistep scheme is constructed and numerical analysis is presented. In Section 1, the mathematical model is stated, and the physical background and related research are introduced. In Section 2, some partition notations and lemmas are stated, and two different (coarse and fine) partitions are defined. In Section 3 and Section 4, we propose the procedures of upwind-block-centered multistep method. The electrostatic potential is solved by a conservative block-centered method, and an approximation of electric field strength with one-order accuracy improvement is shown. An upwind-block-centered multistep scheme is applied to solve the concentration equations and the heat conduction equation. The time derivative is approximated by a multistep method. The diffusion and convection are solved by the block-centered scheme and the upwind scheme, respectively. The composite scheme can solve convection-dominated diffusion problems well because it avoids numerical dispersion and nonphysical oscillation. The concentrations and the temperature and their adjoint vector functions are computed simultaneously. The scheme has the nature of conservation, which is important in the numerical simulation of semiconductor device. In Section 5, we give a theoretical analysis by using the variation, energy estimates, induction hypothesis, embedding theorem and the theory of a priori estimates of differential equations to derive the optimal-order error estimates. In Section 6, numerical experiments are illustrated to show the efficiency and application of this method, and the challenging problem [2, 5–8, 35] can be solved. Several interesting conclusions are obtained.

(I) The method has the physical nature of conservation, which is important in the numerical simulation of semiconductor device, especially in information science. It improves and generalizes the research on numerical simulation in information science [2, 5–10, 35].

(II) The method combines multistep method, block-centered difference and upwind approximation, so it has strong stability and high accuracy and is especially useful in large-scale engineering computations of complicated three-dimensional regions.

(III) The method improves the research on multistep method given by Bramble in [35].

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References

[1] R. Bank, W. Coughran, W. Fichtner, E. Grosse, D. Rose, and R. Smith, *Transient simulation of silicon devices and circuits,* IEEE T. Comput. Aid. D., 4(4) (1985), pp. 436–451.
[2] J. Jerome, Mathematical Theory and Approximation of Semiconductor Models, Philadelphia: SIAM, 1994.
[3] Y. Lou, *On basic semiconductor equation with heat conduction,* J. Partial Differential Equations, 8(1) (1995), pp. 43–54.
[4] Y. Yuan, *Finite difference method and analysis for three-dimensional semiconductor device of heat conduction,* Sci. Sin. Math., 39(11) (1996), pp. 1140–1151.
[5] M. Shi, Physics of Modern Semiconductor Device, Beijing: Science Press, 2002.

[6] Y. HE, AND T. WEI, Computer Simulation Method for Semiconductor Device, Beijing: Sciecence Press, 1989.
[7] Y. YUAN, *Recent progress in numerical methods for semiconductor devices,* Chinese J. Comput. Phys., 26(3) (2009), pp. 317–324.
[8] Y. YUAN, Theory and Application of Reservoir Numerical Simulation, Beijing: Science Press, 2013.
[9] H. GUMMEL, *A self-consistent iterative scheme for one-dimensional steady-state transistor calculation,* IEEE T. Electron. Dev., 11(10) (1964), pp. 455–465.
[10] JR. J. DOUGLAS AND Y. YUAN, *Finite difference methods for the transient behavior of a semiconductor device,* Mat. Apli. Comp., 6(1) (1987), pp. 25–37.
[11] Y. YUAN, L. DING, AND H. YANG, *A new method and theoretical analysis of numerical analog of semiconductor,* Chin. Sci. Bull., 27(7) (1982), pp. 790–795.
[12] Y. YUAN, *Finite element method and analysis of numerical simulation of semiconductor device,* Acta Math. Sci., 13(3) (1993), pp. 241–251.
[13] Y. YUAN, *The approximation of the electronic potential by a mixed method in the simulation of semiconductor,* J. Sys. Sci. Math. Sci., 11(2) (1991), pp. 117–120.
[14] Y. YUAN, *Characteristics method with mixed finite element for transient behavior of semiconductor device,* Chin. Sci. Bull., 36(17) (1991), pp. 1356–1357.
[15] Z. CAI, *On the finite volume element method,* Numer. Math., 58(1) (1991), pp. 713–735.
[16] R. LI, AND Z. CHEN, Generalized Difference of Differential Equations, Changchun: Jilin University Press, 1994.
[17] P. RAVIART AND J. THOMAS, *A mixed finite element method for second order elliptic problems,* in: Mathematical Aspects of the Finite Element Method, Lecture Notes in Mathematics, 606, Springer, 1977.
[18] JR. J. DOUGLAS, R. EWING AND M. WHEELER, *Approximation of the pressure by a mixed method in the simulation of miscible displacement,* RAIRO Anal. Numer., 17(1) (198), pp. 17–33.
[19] JR. J. DOUGLAS, R. EWING AND M. WHEELER, *A time-discretization procedure for a mixed finite element approximation of miscible displacement in porous media,* RAIRO Anal. Numer., 17(3) (1983), pp. 249–265.
[20] T. RUSSELL, *Rigorous block-centered discretization on irregular grids: Improved simulation of complex reservoir systems,* Project Report, Research Corporation, Tulsa, 1995.
[21] A, WEISER, AND M. WHEELER, *On convergence of block-centered finite difference for elliptic problems,* SIAM J. Numer. Anal., 25(2) (1988), pp. 351–375.
[22] J. JONES, A Mixed Volume Method for Accurate Computation of Fluid Velocities in Porous Media, Ph. D. Thesis, University of Colorado, Denver, Co. 1995.
[23] Z. CAI, J. JONES, S. MCCORMILK, AND T. RUSSELL, *Control-volume mixed finite element methods,* Comput. Geosci., 1 (1997), pp. 289–315.
[24] S. CHOU, D. KAWK, AND P. VASSILEVIKI, *Mixed volume methods on rectangular grids for elliptic problem,* SIAM J. Numer. Anal., 37 (2000), pp. 758–771.
[25] S. CHOU, D. KAWK, AND P. VASSILEVIKI, *Mixed volume methods for elliptic problems on trianglar grids,* SIAM J. Numer. Anal., 35 (1998), pp. 1850–1861.
[26] S. CHOU, AND P. VASSILEVIKI, *A general mixed covolume framework for constructing conservative schemes for elliptic problems,* Math. Comput., 68(227) (1999), pp. 991–1011.
[27] H. RUI, AND H. PAN, *A block-centered finite difference method for the Darcy-Forchheimer model,* SIAM J. Numer. Anal., 50(5) (2012), pp. 2612–2631.
[28] H. PAN, AND H. RUI, *Mixed element method for two-dimensional Darcy-Forchheimer model,* J Sci. Comput., 52(3) (2012), pp. 563–587.

[29] Y. YUAN, Y. LIU, C. LI, T. SUN, ANAD L. MA, *Analysis on block-centered finite differences of numerical simulation of semiconductor detector,* Appl., Math. Comput., 279 (2016), pp. 1–15.

[30] Y. YUAN, Q. YANG, C. LI, AND T. SUN, *Numerical method of mixed finite volume-modified upwind fractional step difference for three-dimensional semiconductor device transient behavior problems,* Acta Math. Sci., 37B(1) (2017), pp. 259–279.

[31] T. ARBOGAST, M. WHEELER, AND I. YOTOV, *Mixed finite elements for elliptic problems with tensor coefficients as cell-centered finite differences,* SIAM J. Numer. Anal., 34(2) (1997), pp. 828–852.

[32] T. ARBOGAST, C. DAWSON, P. KEENAN, M. WHEELER, AND I. YOTOV, *Enhanced cell-centered finite differences for elliptic equations on general geometry,* SIAM J. Sci., Comput., 19(2) (1998), pp. 404–425.

[33] J. NITSCHE, *Linear splint-funktionen and die methoden von Ritz for elliptishce randwert probleme,* Arch. Rational Mech. Anal., 36 (1968), pp. 348–355.

[34] L. JIANG, AND Z. PANG, Finite Element Method and Its Theory, Beijing: People's Education Press, 1979.

[35] J. BRAMBLE, R. EWING, AND G. LI, *Alternating direction multistep methods for parabolic problems iterative stabilization,* SIAM J. Numer., Anal., 26(4) (1989), pp. 904–919.