

三维热传导型半导体器件瞬态模拟问题的 Crank-Nicolson 差分 - 流线扩散 有限元法及其数值分析*

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摘要 本文研究三维热传导型半导体器件瞬态模拟问题的数值方法. 针对数学模型中各方程不同的特点, 分别提出不同的有限元格式. 特别针对浓度方程组是对流为主扩散问题的特点, 使用 Crank-Nicolson 差分 - 流线扩散计算格式, 提高了数值解的稳定性. 得到的 L^2 误差估计关于空间剖分步长是拟最优的, 关于时间步长具有二阶精度.

关键词 半导体, 三维热传导, Crank-Nicolson 格式, 差分流线扩散法, 误差估计

1 引言

三维热传导型半导体器件瞬态问题的数学模型是由四个方程组成的非线性偏微分方程组的初边值问题^[1]:

$$-\Delta\psi = \nabla \cdot u = \alpha(p - e + N(x)), \quad (1.1)$$

$$\frac{\partial e}{\partial t} = \nabla \cdot (D_e(x)\nabla e - \mu_e(x)e\nabla\psi) - R(e, p, T), \quad (1.2)$$

$$\frac{\partial p}{\partial t} = \nabla \cdot (D_p(x)\nabla p + \mu_p(x)p\nabla\psi) - R(e, p, T), \quad (1.3)$$

$$\rho(x)\frac{\partial T}{\partial t} - \Delta T = [D_p(x)\nabla p + \mu_p p \nabla\psi - (D_e(x)\nabla e - \mu_e e \nabla\psi)] \cdot \nabla\psi, \quad (1.4)$$

$$x = (x_1, x_2, x_3)^T \in \Omega, \quad t \in J = (0, \bar{T}].$$

初始条件:

$$e(x, 0) = e_0(x), \quad p(x, 0) = p_0(x), \quad T(x, 0) = T_0(x), \quad x \in \Omega. \quad (1.5)$$

边界条件:

$$\psi = e = p = T = 0, \quad (x, t) \in \partial\Omega \times J. \quad (1.6)$$

这里 $\Omega \subset R^3$ 为具有逐片光滑边界的有界区域, \bar{T} 为一给定正数. 我们只考虑齐次边界条件, 非齐次边界条件可以化为齐次的情形. 方程中的未知函数是电场位势 ψ , 电子和

本文 2000 年 1 月 28 日收到.

* 国家重点基础研究规划项目 (G1999032803) 和教育部高等院校骨干教师专项科研基金资助项目.

空穴浓度 e 和 p 与温度函数 T . 方程组 (1.1)–(1.4) 中出现的系数均有正的上界和下界, $\alpha = \frac{q}{\epsilon}$, q 和 ϵ 表示电子负荷和介电系数, 均为正常数, $D_e(x)$ 和 $D_p(x)$ 为扩散系数, $\mu_e(x)$ 和 $\mu_p(x)$ 为电子和空穴的迁移率, 并且有关系 $D_s(x) = U_T \mu_s(x)$, $s = e, p$. U_T 是热量. $N(x) = N_D(x) - N_A(x)$ 是给定的函数, $N_D(x)$ 和 $N_A(x)$ 分别是施主和受主杂质浓度. $R(e, p, T)$ 是电子和空穴在考虑温度效应下产生的复合率. $R(e, p, T)$ 关于三个变量是 Lipschitz 连续的.

关于半导体器件数值模拟已有不少的工作. 最早 Gummel 于 1964 年提出用序列迭代法计算这类问题 [2]. 其后, Douglas 和袁益让等 [3,4] 对一维和二维简单模型 (不考虑温度效应和常系数) 提出了便于数值计算的差分格式. 实际上, 考虑三维域上具有温度效应的数学模型才能更真实地反应半导体器件的瞬态行为. 袁益让 [1] 提出了热传导型半导体器件瞬态模拟问题的特征差分格式. 羊丹平 [5] 提出了对称正定混合元方法. 本文针对各个方程不同的特点分别提出不同的有限元格式. 从 (1.1)–(1.4) 可以看出电场位势 ψ 是通过电场强度 $u = -\nabla\psi$ 出现在电子和空穴浓度方程以及温度方程中的. 为了高精度逼近 u , 对 (1.1) 我们使用混合元方法求解. 考虑到电子和空穴浓度方程是对流为主的扩散方程这一显著特点, 我们提出差分 - 流线扩散有限元法, 对时间的离散使用 Crank-Nicolson 格式. Streamline-Difusion method (SD 方法) 是由 Hughes 和 Brooks 于 1980 年前后提出的求解定常的对流占优和对流扩散问题的有限元方法. SD 方法兼具良好的数值稳定性和高阶精度, 因此越来越受到重视. 以往的文献常常采用时空有限元, 这样增加了数值计算的复杂性. 张强和孙澈等 [6] 对发展型的二维非线性对流扩散方程提出差分 - 流线扩散法 (FSDS 方法) 并得到拟最优的 L^2 收敛性估计, 同时 [6] 还给出了数值算例. 但时间上仅具有一阶精度, 本文使用 C-N 格式, 最后的 L^2 估计具有二阶时间精度, 因此可取较大的时间步长.

对文中出现的记号做一些必要的说明: (\cdot, \cdot) 表示 $L^2(\Omega)$ 或 $L^2(\Omega)^3$ 空间的内积. 如果 $\phi = (\phi_1, \phi_2, \phi_3)^T$, 定义 $\|\phi\| = \|\phi\|_{L^2} = (\|\phi_1\|^2 + \|\phi_2\|^2 + \|\phi_3\|^2)^{1/2}$. $W^{m,p}(\Omega)$ 表示通常的 Sobolev 空间. 如果 $p = 2$ 简记为 $H^m(\Omega)$, 其范数记为 $\|\cdot\|_m$. 设 H 是一赋范线性空间, W 定义在 $[a, b] \times \Omega$ 上. 如果 $t \in [a, b]$, $W(\cdot, t) \in H$, 并且 $\|W\|_H \in L^p([a, b])$, 则称 $W \in L^p(a, b; H)$, $0 \leq p \leq \infty$, 定义 $\|W\|_{L^p(a,b;H)} = \|F(t)\|_{L^p([a,b])}$, 其中 $F(t) = \|W\|_H(t)$. 文中简记为 $\|\cdot\|_{L^p(H)}$. 记

$$\phi^n = \phi(x, t^n), \quad \phi^{n+\frac{1}{2}} = \phi(x, t^{n+\frac{1}{2}}), \quad \bar{\phi}^{n+\frac{1}{2}} = \frac{\phi^{n+1} + \phi^n}{2}, \quad \bar{d}_t \phi^{n+\frac{1}{2}} = \frac{\phi^{n+1} - \phi^n}{\Delta t},$$

这里 Δt 是时间步长.

对问题的精确解及系数作如下假定:

(R1) 问题 (1.1)–(1.6) 有唯一解, 且

$$e, p, T, e_0, p_0, T_0 \in H^{r+1}(\Omega) \cap H_0^1(\Omega), \quad \nabla \frac{\partial^2 s}{\partial t^2}, \Delta \frac{\partial^2 s}{\partial t^2}, \frac{\partial^3 u}{\partial t^3} \in L^2(L^2), \quad u \in (W^{r,\infty})^3,$$

$$\frac{\partial s}{\partial t}, \frac{\partial T}{\partial t}, \frac{\partial u}{\partial t} \in L^2(H^{r+1}), \quad \frac{\partial^2 s}{\partial t^2}, \frac{\partial^2 T}{\partial t^2}, \frac{\partial^2 u}{\partial t^2} \in L^2(L^2),$$

$$\psi \in H^{r+3}, \quad \|s\|_\infty \leq s^*, \quad \|u\|_\infty \leq u^*, \quad s = e, p.$$

(C1) 问题 (1.1)–(1.6) 的系数有正的上界和下界: $0 < D_{s,*} \leq D_s(x) \leq D_s^*$, $0 < \mu_{s,*} \leq \mu_s \leq \mu_s^*$, $|\nabla \mu_s| \leq \mu_{s,1}$, $s = e, p$, $0 < \mu_{s,*} \leq \mu_s \leq \mu_s^*$.

在第 2 节, 我们给出问题 (1.1)–(1.6) 的 C-N FSDS 计算格式. 在第 3 至第 5 节, 研究格式的可解性和收敛性.

2 C-N FSDS 计算格式

设 $T_h = \{\tau_k\}$ 为 Ω 的拟一致正则剖分族, 相应的网格参数为 $0 < h \leq h_0 < 1$. 定义有限元空间: $S_h = \{v \in H_0^1; v|_{\tau_k} \in P_r(\tau_k), \forall \tau_k \in T_h\}$. S_h 具有下面的逼近性质和逆性质: 存在 $C_0 > 0$, 使得

$$\inf_{v_h \in S_h} (\|v - v_h\| + h\|\nabla(v - v_h)\|) \leq C_0 \|v\|_{r+1} h^{r+1}, \quad \forall v \in H_0^1 \cap H^{r+1}; \quad (\text{A1})$$

$$\begin{aligned} \|\nabla v_h\| &\leq C_0 h^{-1} \|v_h\|, & \|v_h\|_\infty &\leq C_0 h^{-\frac{3}{2}} \|v_h\|, \\ \sum_{\tau_k \in T_h} \int_{\partial\tau_k} |v_h|^2 ds &\leq C_0 h^{-1} \|v_h\|^2, & \forall v_h \in S_h. \end{aligned} \quad (\text{I1})$$

定义指数为 r 的 Raviart-Thomas^[7] 或 Nedelec^[8] 混合元空间 $\widetilde{V}_h \times \widetilde{W}_h$. 令 $V_h = \widetilde{V}_h$, $W_h = \widetilde{W}_h / \{\phi = \text{常数}\}$. $V_h \times W_h$ 有如下的逼近性质: 存在 $C_1 \geq 0$,

$$\begin{aligned} \inf_{v_h \in V_h} \|v - v_h\| &\leq C_1 \|v\|_{H^{r+1}(\Omega)} h^{r+1}, & \forall v \in H^{r+1}(\Omega)^3; \\ \inf_{v_h \in V_h} \|v - v_h\|_{H(\text{div}; \Omega)} &\leq C_1 \|v\|_{H^{r+2}(\Omega)} h^{r+1}, & \forall v \in H^{r+2}(\Omega)^3; \\ \inf_{w_h \in W_h} \|w - w_h\| &\leq C_1 \|w\|_{H^{r+1}(\Omega)} h^{r+1}, & \forall w \in H^{r+1}(\Omega). \end{aligned} \quad (\text{A2})$$

同时 $V_h \times W_h$ 还具有类似于 (I1) 的逆性质, 其中的常数也记为 C_0 .

作时间剖分: $0 = t^0 < t^1 < \dots < t^N = \bar{T}$, $\Delta t = \bar{T}/N$. 记 $t^n = n\Delta t$, $t^{n+\frac{1}{2}} = (n+\frac{1}{2})\Delta t$.

将方程组 (1.1)–(1.4) 改为下面的形式:

$$-\Delta\psi = \nabla \cdot u = \alpha(p - e + N(x)), \quad (2.1)$$

$$\frac{\partial e}{\partial t} - \mu_e u \cdot \nabla e - \nabla \cdot (D_e \nabla e) = eu \cdot \nabla \mu_e + \alpha \mu_e e(p - e + N) - R(e, p, T), \quad (2.2)$$

$$\frac{\partial p}{\partial t} + \mu_p u \cdot \nabla p - \nabla \cdot (D_p \nabla p) = -pu \cdot \nabla \mu_p - \alpha \mu_p p(p - e + N) - R(e, p, T), \quad (2.3)$$

$$\rho(x) \frac{\partial T}{\partial t} - \Delta T = u \cdot (D_e \nabla e - D_p \nabla p) + u \cdot u (\mu_p p - \mu_e e). \quad (2.4)$$

由 (2.1)–(2.4) 的变分形式易得 C-N FSDS 格式: 求 $\{u_h^n, \psi_h^n, e_h^n, p_h^n, T_h^n\} \subset V_h \times W_h \times S_h \times S_h \times S_h$:

$$\begin{aligned} &(\bar{d}_t e_h^{n+\frac{1}{2}} - \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{e}_h^{n+\frac{1}{2}}, v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) + (D_e \nabla \bar{e}_h^{n+\frac{1}{2}}, \nabla v_h) \\ &+ (\nabla \cdot (D_e \nabla \bar{e}_h^{n+\frac{1}{2}}), \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) \\ &= (\bar{e}_h^{n+\frac{1}{2}} \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \mu_e + \alpha \mu_e \bar{e}_h^{n+\frac{1}{2}} (\widehat{p}_h^{n+\frac{1}{2}} - \bar{e}_h^{n+\frac{1}{2}} + N) - R(\bar{e}_h^{n+\frac{1}{2}}, \widehat{p}_h^{n+\frac{1}{2}}, \widehat{T}_h^{n+\frac{1}{2}}), \\ &v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h), \quad \forall v_h \in S_h, \quad n \geq 0; \end{aligned} \quad (2.5)$$

$$\begin{aligned} &(\bar{d}_t p_h^{n+\frac{1}{2}} + \mu_p \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{p}_h^{n+\frac{1}{2}}, v_h + \delta_p \mu_p \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) + (D_p \nabla \bar{p}_h^{n+\frac{1}{2}}, \nabla v_h) \\ &- (\nabla \cdot (D_p \nabla \bar{p}_h^{n+\frac{1}{2}}), \delta_p \mu_p \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) \\ &= -(\bar{p}_h^{n+\frac{1}{2}} \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \mu_p + \alpha \mu_p \bar{p}_h^{n+\frac{1}{2}} (\widehat{p}_h^{n+\frac{1}{2}} - \bar{e}_h^{n+\frac{1}{2}} + N) + R(\bar{e}_h^{n+\frac{1}{2}}, \widehat{p}_h^{n+\frac{1}{2}}, \widehat{T}_h^{n+\frac{1}{2}}), \\ &v_h + \delta_p \mu_p \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h), \quad \forall v_h \in S_h, \quad n \geq 0; \end{aligned} \quad (2.6)$$

$$\begin{aligned}
 & (\rho \bar{d}_t T_h^{n+\frac{1}{2}}, v_h) + (\nabla \bar{T}_h^{n+\frac{1}{2}}, \nabla v_h) \\
 & = (\hat{u}_h^{n+\frac{1}{2}} (D_e \nabla \bar{e}_h^{n+\frac{1}{2}} - D_p \nabla \bar{p}_h^{n+\frac{1}{2}}) + \hat{u}_h^{n+\frac{1}{2}} \cdot \hat{u}_h^{n+\frac{1}{2}} (\mu_p \bar{p}_h^{n+\frac{1}{2}} - \mu_e \bar{e}_h^{n+\frac{1}{2}}), v_h), \\
 & \quad \forall v_h \in S_h, \quad n \geq 0; \tag{2.7}
 \end{aligned}$$

$$(\nabla \cdot u_h^{n+1}, \phi) = (\alpha(p_h^{n+1} - e_h^{n+1} + N), \phi), \quad \forall \phi \in W_h, \tag{2.8}$$

$$(u_h^{n+1}, w_h) - (\psi_h^{n+1}, \nabla \cdot w_h) = 0, \quad \forall w_h \in V_h, \quad n \geq 0; \tag{2.9}$$

$$e_h^0 = \Pi_h e_0(x), \quad p_h^0 = \Pi_h p_0(x), \quad T_h^0 = P_1 T_0(x), \tag{2.10}$$

其中

$$(\nabla \cdot (D_s \nabla \bar{e}_h^{n+\frac{1}{2}}), \delta_s \mu_s \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla v) = \sum_{\tau_k \in T_h} (\nabla \cdot (D_s \nabla \bar{s}_h^{n+\frac{1}{2}}), \delta_s \mu_s \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla v)_{\tau_k}, \quad s = e, p.$$

$\hat{s}_h^{n+\frac{1}{2}}$ 定义为: 对 $s = e, p, T$ 和 u

$$\hat{s}_h^{n+\frac{1}{2}} = \begin{cases} \frac{3}{2} s_h^n - \frac{1}{2} s_h^{n-1}, & n \geq 1, \\ s_0 + \frac{\Delta t}{2} s_{ht}^0, & n = 0. \end{cases}$$

如果 $n = 0$, u_0 改为 u_h^0 . $\{u_h^0, \psi_h^0\} \subset V_h \times W_h$ 定义如下:

$$(\nabla \cdot u_h^0, \phi_h) = (\alpha(p_0 - e_0 + N), \phi_h), \quad \forall \phi_h \in W_h, \tag{2.11}$$

$$(u_h^0, w_h) - (\psi_h^0, \nabla \cdot w_h) = 0, \quad \forall w_h \in V_h. \tag{2.12}$$

Π_h 为有限元空间的插值算子, P_1 为椭圆投影算子. δ_e 和 δ_p 为人为选定的小参数 (见第 5 节).

定义

$$e_{ht}^0 = \mu_e u_h^0 \cdot \nabla e_0 + \nabla \cdot (D_e \nabla e_0) + e_0 u_h^0 \cdot \nabla \mu_e + \alpha \mu_e e_0 (p_0 - e_0 + N) - R(e_0, p_0, T_0), \tag{2.13}$$

$$\begin{aligned}
 p_{ht}^0 & = -\mu_p u_h^0 \cdot \nabla p_0 + \nabla \cdot (D_p \nabla p_0) \\
 & \quad - p_0 u_h^0 \cdot \nabla \mu_p - \alpha \mu_p p_0 (p_0 - e_0 + N) - R(e_0, p_0, T_0), \tag{2.14}
 \end{aligned}$$

$$T_{ht}^0 = \frac{1}{\rho(x)} [\Delta T_0 + u_h^0 (D_e \nabla e_0 - D_p \nabla p_0) + u_h^0 \cdot u_h^0 (\mu_p p_0 - \mu_e e_0)]. \tag{2.15}$$

(2.1) 的两边关于 t 求导数, 并令 $t = 0$. 用混合元方法求 $\{u_{ht}^0, \psi_{ht}^0\} \subset V_h \times W_h$:

$$(\nabla \cdot u_{ht}^0, \phi_h) = (\alpha(p_{ht}^0 - e_{ht}^0), \phi_h), \quad \forall \phi_h \in W_h; \tag{2.16}$$

$$(u_{ht}^0, w_h) - (\psi_{ht}^0, \nabla \cdot w_h) = 0, \quad \forall w_h \in V_h. \tag{2.17}$$

C-N FSDS 计算格式的计算顺序为: 首先由插值算子和椭圆投影算子计算出 e_h^0, p_h^0 和 T_h^0 . 再由 (2.11)-(2.17) 依次求出 $u_h^0, \psi_h^0, e_{ht}^0, p_{ht}^0, T_{ht}^0, u_{ht}^0$ 和 ψ_{ht}^0 . 再按定义计算 $\hat{s}_h^{\frac{1}{2}}$, $s = e, p, T$ 和 u . 然后就可以按格式 (2.5)-(2.9) 求解, 其中 (2.5) 和 (2.6) 可以同时计算.

3 C-N FSDS 格式的可解性

记 $q_s = D_s^*/D_{s,*}$ 和 $d_s = D_s^*/h_0$, $s = e, p$. 文中出现的 $C_i, K, \tilde{K}, \tilde{C}$ 和 M 等均为与 $h, \Delta t, 1/D_{e,*}$ 和 $1/D_{p,*}$ 无关的正常数, 在不同的地方代表不同的值, ε 为一般的小正数.

定理 1 假定 $\|\hat{u}_h^{n+\frac{1}{2}}\|_\infty \leq 2K^*$, 参数 δ_e 和 δ_p 满足

$$\delta_s \leq \frac{h}{16q_s K^* (3\mu_s^* C_0 + \mu_{s,1} h_0)}, \quad s = e, p; \quad (3.1)$$

并且时间步长满足

$$\Delta t = dh^{1+\sigma}, \quad (3.2)$$

d 为一适当大的正数, σ 为一小正数. 则当 h 适当小时, (2.5)–(2.10) 有唯一解.

证 由 Brezzi 定理^[9], 不难推出 (2.9) 和 (2.10) 的混合元解存在. 再由系数的正定性易知 (2.8) 的有限元解存在唯一. 因此只需考虑 (2.5) 和 (2.6) 的可解性. 下面只就 (2.5) 来证明. 记 $U = \hat{u}_h^{n+\frac{1}{2}}$. (2.5) 的可解性等价于下面的齐次方程

$$\begin{aligned} & (2W - \Delta t \mu_e U \cdot \nabla W, v_h - \delta_e \mu_e U \cdot \nabla v_h) + \Delta t (D_e \nabla W, \nabla v_h) \\ & + \Delta t (\nabla \cdot (D_e \nabla W), \delta_e \mu_e U \cdot \nabla v_h) = 0, \quad \forall v_h \in S_h \end{aligned} \quad (3.3)$$

只有零解. 在 (3.3) 中令 $v_h = W$, 并逐项估计. 注意到 $\delta_e q_e \mu_e^* K^* C_0 h^{-1} \leq \frac{1}{48}$,

$$\Delta t (\mu_e U \cdot \nabla W, W) \leq 2K^* \mu_e^* C_0 d h^\sigma \|W\|^2 \leq \tilde{C} h^\sigma \|W\|^2, \quad (3.4)$$

$$\delta_e (\mu_e U \cdot \nabla W, 2W) \leq 2K^* \mu_e^* C_0 \delta_e h^{-1} \|W\|^2 \leq \frac{1}{12} \|W\|^2, \quad (3.5)$$

$$(\nabla \cdot (D_e \nabla W), \delta_e \mu_e U \cdot \nabla W) = I_1 + I_2 + I_3. \quad (3.6)$$

注意到

$$I_1 = - \sum_{\tau_k \in T_h} (D_e \nabla W, \delta_e \operatorname{div}(\mu_e U) \nabla W)_{\tau_k} \leq D_{e,*} q \delta_e (2\mu_e^* K^* C_0 h^{-1} + 2K^* \mu_{e,1}) \|\nabla W\|^2,$$

$$I_2 = - \sum_{\tau_k \in T_h} (D_e \nabla W, \delta_e \mu_e U \Delta W)_{\tau_k} \leq 2D_{e,*} q \delta_e \mu_e^* K^* C_0 h^{-1} \|\nabla W\|^2,$$

$$I_3 = \sum_{\tau_k \in T_h} \int_{\partial \tau_k} D_e \nabla W \cdot \nu \delta_e \mu_e U \cdot \nabla W \, ds \leq 2q_e K^* D_{e,*} \mu_e^* C_0 h^{-1} \|\nabla W\|^2,$$

这里 ν 是 $\partial \tau_k$ 的单位法向量. 于是

$$I_1 + I_2 + I_3 \leq (6q \mu_e^* K^* C_0 h^{-1} + 2q \mu_{e,1} K^*) \delta_e D_{e,*} \|\nabla W\|^2 \leq \frac{1}{8} D_{e,*} \|\nabla W\|^2. \quad (3.7)$$

结合 (3.4)–(3.7) 及方程 (3.3):

$$\left(\frac{23}{12} - \tilde{C} h^\sigma \right) \|W\|^2 + \delta_e \Delta t \|\mu_e U \cdot \nabla W\|^2 + \frac{7}{8} D_{e,*} \Delta t \|\nabla W\|^2 \leq 0. \quad (3.8)$$

所以, 当 h 适当小时 $W = 0$. 定理 1 证毕.

上述定理中的假定 $\|\hat{u}_h^{n+\frac{1}{2}}\|_\infty \leq 2K^*$ 将在第五节中得到验证.

4 几个投影

为了得到最后的误差估计, 本节引入几个有用的投影. 考虑映射 $\{\tilde{u}_h, \tilde{\psi}_h\} : J \mapsto V_h \times W_h$ 满足:

$$(\nabla \cdot \tilde{u}_h, \phi_h) = (\alpha(e - p + N), \phi_h), \quad \forall \phi_h \in W_h, \quad (4.1)$$

$$(\tilde{u}_h, v_h) - (\tilde{\psi}_h, \nabla \cdot v_h) = 0, \quad \forall v_h \in V_h. \quad (4.2)$$

由 Breezi 定理及 (ψ, u) 的光滑性, 对 $t \in J$, 成立估计:

$$\|\tilde{u}_h - u\|_{H(\text{div}; \Omega)} + \|\tilde{\psi}_h - \psi\| \leq M\|\psi\|_{H^{r+3}(\Omega)}h^{r+1}. \quad (4.3)$$

由 [12] 的定理 3.1, 我们有

$$\|\tilde{u}_h - u\|_{L^\infty} \leq M\|u\|_{W^{r,\infty}}h^r. \quad (4.4)$$

对电子和空穴浓度方程引入插值算子 Π_h , 记 $\eta_s = s^n - \Pi_h s^n$, $s = e, p$. 根据有限元空间的插值理论^[10], 对 $s = e, p$ 成立:

$$\begin{aligned} \|\eta_s^n\| + h\|\nabla\eta_s^n\| &\leq M\|s^n\|_{r+1}h^{r+1}, & n = 0, 1, \dots, N; \\ \|\bar{d}_t\eta_s^{n+\frac{1}{2}}\|^2 &\leq M(\Delta t)^{-1}h^{2r+2}\|s_t\|_{L^2(t^n, t^{n+1}; H^{r+1}(\Omega))}^2, & n = 0, 1, \dots, N-1; \\ \|\eta_s^n\|_\infty &\leq M\|s\|_{r+1}h^{r-\frac{1}{2}}, & n = 0, 1, \dots, N. \end{aligned} \quad (4.5)$$

根据迹不等式和内插空间理论^[11]:

$$\sum_{\tau_k \in T_h} \int_{\partial\tau_k} |\nabla\eta_s^n|^2 ds \leq Mh^{2r-1}\|s^n\|_{r+1}^2, \quad n = 0, 1, \dots, N. \quad (4.6)$$

对温度变量, 引入椭圆投影: $P_1 : J \mapsto S_h$ 满足

$$(\nabla(P_1 T - T), \nabla v_h) = 0, \quad \forall v_h \in S_h. \quad (4.7)$$

记 $\eta_T = T - P_1 T$. 根据椭圆方程有限元理论^[10], 成立逼近估计:

$$\|\eta_T\| + h\|\nabla\eta_T\| \leq M\|T\|_{r+1}h^{r+1}. \quad (4.8)$$

5 误差估计

本节我们分析 C-N SDFD 计算格式的收敛性. 记

$$\begin{aligned} \xi_s^n &= s_h^n - \Pi_h s^n, & \eta_s^n &= s^n - \Pi_h s^n, & \varepsilon_s^n &= s_h^n - s^n = \xi_s^n - \eta_s^n, & s &= e, p, \\ \xi_T^n &= T_h^n - P_1 T^n, & \eta_T^n &= T^n - P_1 T^n, & \varepsilon_T^n &= T_h^n - T^n = \xi_T^n - \eta_T^n, \\ \xi_u^n &= u_h^n - \tilde{u}_h^n, & \eta_u^n &= u^n - \tilde{u}_h^n, & \varepsilon_h^n &= u_h^n - u^n = \xi_u^n - \eta_u^n. \end{aligned}$$

定理 2 假定 $r \geq 2$, 条件 (R1) 和 (C1) 成立, 参数 δ_s ($s = e, p$) 满足

$$\delta_s = \min \{C_{2s}h, D_{s,*}^{-1}C_{3s}h^2\}, \quad (5.1)$$

其中 C_{2s}, C_{3s} 满足:

$$C_{2s}(3q_s\mu_s^*C_0u^* + q_s\mu_{s,1}u^*h_0) \leq \frac{1}{16}, \quad (5.2)$$

$$C_{3s}(q_s^2\mu_s^*u^{*2}d_s^{-2} + 8q_s^2C_0^2) \leq \frac{1}{2}, \quad (5.3)$$

并且时间步长 Δt 满足 (3.2), 则问题 (1.1)–(1.6) 的 C-N FSD 格式有下面的误差估计:

$$\begin{aligned}
 & \max_{1 \leq n \leq N} \|\varepsilon_u^n\|^2 + \max_{1 \leq n \leq N} \|\varepsilon_e^n\|^2 + \max_{1 \leq n \leq N} \|\varepsilon_p^n\|^2 + \max_{1 \leq n \leq N} \|\varepsilon_T^n\|^2 \\
 & + \sum_{n=0}^{N-1} [\delta_e \|\mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\varepsilon}_e^{n+\frac{1}{2}}\|^2 + \delta_p \|\mu_p \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\varepsilon}_p^{n+\frac{1}{2}}\|^2] \Delta t \\
 & + \sum_{n=0}^{N-1} [D_{e,*} \|\nabla \bar{\varepsilon}_e^{n+\frac{1}{2}}\|^2 + D_{p,*} \|\nabla \bar{\varepsilon}_p^{n+\frac{1}{2}}\|^2 + \|\nabla \bar{\varepsilon}_T^{n+\frac{1}{2}}\|^2] \Delta t \\
 & + \sum_{n=0}^{N-1} [\delta_e \|d_t \varepsilon_e^{n+\frac{1}{2}}\|^2 + \delta_p \|d_t \varepsilon_p^{n+\frac{1}{2}}\|^2] \Delta t \\
 & \leq M \{ D_{e,*} h^{2r} + D_{p,*} h^{2r} + h^{2r+1} + (\Delta t)^4 \}. \tag{5.4}
 \end{aligned}$$

证 由 (2.11) 和 (2.12), 利用 Breezi 定理, 我们有估计

$$\|u_h^0 - u^0\| \leq M \|\psi^0\|_{H^{r+3}(\Omega)} h^{r+1}. \tag{5.5}$$

由 (2.8), (2.9), (4.1) 和 (4.2) 得电场位势的误差方程, 当 $n \geq 0$ 时,

$$(u_h^{n+1} - \widetilde{u}_h^{n+1}, v_h) - (\psi_h^{n+1} - \widetilde{\psi}_h^{n+1}, \nabla \cdot v_h) = 0, \quad \forall v_h \in V_h; \tag{5.6}$$

$$(\nabla \cdot (u_h^{n+1} - \widetilde{u}_h^{n+1}), \phi_h) = (\alpha(\varepsilon_e^{n+1} - \varepsilon_p^{n+1}), \phi_h), \quad \forall \phi_h \in W_h. \tag{5.7}$$

由 Breezi 定理^[9]:

$$\|u_h^{n+1} - \widetilde{u}_h^{n+1}\| + \|\psi_h^{n+1} - \widetilde{\psi}_h^{n+1}\| \leq M(\|\varepsilon_e^{n+1}\| + \|\varepsilon_p^{n+1}\|). \tag{5.8}$$

结合 (4.3) 及 (4.5) 则有

$$\|u^{n+1} - u_h^{n+1}\| + \|\psi^{n+1} - \psi_h^{n+1}\| \leq M(h^{r+1} + \|\xi_e^{n+1}\| + \|\xi_p^{n+1}\|). \tag{5.9}$$

参照 [6] 记:

$$\begin{aligned}
 B_n(\bar{w}^{n+\frac{1}{2}}, v) &= (\bar{d}_t w^{n+\frac{1}{2}} - \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{w}^{n+\frac{1}{2}}, v - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v) \\
 &+ (D_e \nabla \bar{w}^{n+\frac{1}{2}}, \nabla v) + (\nabla \cdot (D_e \nabla \bar{w}^{n+\frac{1}{2}}), \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v),
 \end{aligned}$$

易得电子浓度的误差方程:

$$\begin{aligned}
 & B_n(\bar{\xi}_e^{n+\frac{1}{2}}, v_h) \\
 = & B_n(\bar{\xi}_e^{n+\frac{1}{2}}, v_h) + (e_t^{n+\frac{1}{2}} - d_t e^{n+\frac{1}{2}}, v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) \\
 & + (\mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{e}^{n+\frac{1}{2}} - \mu_e u^{n+\frac{1}{2}} \cdot \nabla e^{n+\frac{1}{2}}, v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) \\
 & + (D_e (\nabla e^{n+\frac{1}{2}} - \nabla \bar{e}^{n+\frac{1}{2}}), v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) \\
 & + (\nabla \cdot (D_e \nabla (e^{n+\frac{1}{2}} - \bar{e}^{n+\frac{1}{2}})), \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) \\
 & + (\widehat{e}_h^{n+\frac{1}{2}} \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \mu_e - e^{n+\frac{1}{2}} u^{n+\frac{1}{2}} \cdot \nabla \mu_e, v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h) \\
 & + (\alpha \mu_e \widehat{e}_h^{n+\frac{1}{2}} (\widehat{p}_h^{n+\frac{1}{2}} - \widehat{e}_h^{n+\frac{1}{2}} + N) - \alpha \mu_e e^{n+\frac{1}{2}} (p^{n+\frac{1}{2}} - e^{n+\frac{1}{2}} + N), v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h)
 \end{aligned}$$

$$+ (R(e^{n+\frac{1}{2}}, p^{n+\frac{1}{2}}, T^{n+\frac{1}{2}}) - R(\widehat{e}_h^{n+\frac{1}{2}}, \widehat{p}_h^{n+\frac{1}{2}}, \widehat{T}_h^{n+\frac{1}{2}}), v_h - \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla v_h), \quad \forall v_h \in S_h. \quad (5.10)$$

当 $n \geq 1$ 时, 对 $s = e, p, T$,

$$\begin{aligned} \|\widehat{s}_h^{n+\frac{1}{2}} - s^{n+\frac{1}{2}}\|^2 &\leq M \left\{ \|\varepsilon_s^n\|^2 + \|\varepsilon_s^{n-1}\|^2 + (\Delta t)^3 \left\| \frac{\partial^2 s}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right\} \\ &\leq M \left\{ h^{2r+2} + \|\xi_s^n\|^2 + \|\xi_s^{n-1}\|^2 + (\Delta t)^3 \left\| \frac{\partial^2 s}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right\}, \end{aligned} \quad (5.11)$$

和

$$\begin{aligned} \|\widehat{u}_h^{n+\frac{1}{2}} - u^{n+\frac{1}{2}}\|^2 &\leq M \left\{ h^{2r+2} + \|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 \right. \\ &\quad \left. + (\Delta t)^3 \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right\}. \end{aligned} \quad (5.12)$$

当 $n = 0$ 时, 注意到 (2.13)-(2.15), 对 $s = e, p, T$, 成立

$$\begin{aligned} \|\widehat{s}^{\frac{1}{2}} - s^{\frac{1}{2}}\|^2 &\leq 2 \left[\left\| \frac{\Delta t}{2} (s_{ht}^0 - s_t^0) \right\|^2 + \left\| \int_0^{t^{\frac{1}{2}}} (t^{\frac{1}{2}} - t) \frac{\partial^2 s}{\partial t^2} \right\|^2 \right] \\ &\leq M \left\{ \|u^0 - u_h^0\|^2 + (\Delta t)^3 \left\| \frac{\partial^2 s}{\partial t^2} \right\|_{L^2(0, t^{\frac{1}{2}}; L^2)}^2 \right\} \\ &\leq M \left\{ h^{2r+2} + (\Delta t)^3 \left\| \frac{\partial^2 s}{\partial t^2} \right\|_{L^2(0, t^{\frac{1}{2}}; L^2)}^2 \right\}, \end{aligned} \quad (5.13)$$

和

$$\begin{aligned} \|u_h^{\frac{1}{2}} - u^{\frac{1}{2}}\|^2 &\leq M \left\{ \|u_h^0 - u^0\|^2 + (\Delta t)^2 \|u_{ht}^0 - u_t^0\|^2 + (\Delta t)^3 \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(0, t^{\frac{1}{2}}; L^2)}^2 \right\} \\ &\leq M \left\{ h^{2r+2} + (\Delta t)^3 \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(0, t^{\frac{1}{2}}; L^2)}^2 \right\}. \end{aligned} \quad (5.14)$$

作归纳假定:

$$\begin{aligned} \text{(a)} \quad &\|\widehat{u}_h^{n+\frac{1}{2}} - u^{n+\frac{1}{2}}\|_\infty \leq \widetilde{K} h^{\frac{1}{2}}, \quad \|\widehat{u}_h^{n+\frac{1}{2}}\|_\infty \leq 2u^*, \quad n = 0, 1, \dots, N-1; \\ \text{(b)} \quad &\|\widehat{s}_h^{n+\frac{1}{2}}\|_\infty \leq 3s^*, \quad s = e, p. \end{aligned} \quad (5.15)$$

实际上, 对 $s = e$ 和 p , $D_{s,*}^{-1} \leq q_s d_s^{-1} h^{-1}$. 所以存在与 $D_{s,*}^{-1}$ 无关的常数 C_{4s} 使得 $\delta_s \leq C_{4s} h$. 在误差方程 (5.10) 中, 令 $v_h = \overline{\xi}_e^{n+\frac{1}{2}}$, 右端后七项依次记为 $Q_1 \sim Q_7$. 注意到 $D_{e,*}^{-1} \leq q_e d_e^{-1} h^{-1}$, 逐项估计 $Q_1 \sim Q_7$, 我们有:

$$\begin{aligned} (dt \xi_e^{n+\frac{1}{2}}, \overline{\xi}_e^{n+\frac{1}{2}}) &= \frac{1}{2\Delta t} (\|\xi_e^{n+1}\|^2 - \|\xi_e^n\|^2), \\ (dt \xi_e^{n+\frac{1}{2}}, \delta_e \mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \overline{\xi}_e^{n+\frac{1}{2}}) &\leq \frac{\delta_e}{2} \|\mu_e \widehat{u}_h^{n+\frac{1}{2}} \cdot \nabla \overline{\xi}_e^{n+\frac{1}{2}}\|^2 + \frac{\delta_e}{2} \|\overline{d}_t \xi_e^{n+\frac{1}{2}}\|^2, \\ (\mu_e u^{n+\frac{1}{2}} \cdot \nabla \overline{\xi}_e^{n+\frac{1}{2}}, \overline{\xi}_e^{n+\frac{1}{2}}) &= -\frac{1}{2} (\overline{\xi}_e^{n+\frac{1}{2}}, \nabla \cdot (\mu_e u^{n+\frac{1}{2}}) \overline{\xi}_e^{n+\frac{1}{2}}) \leq M \|\overline{\xi}_e^{n+\frac{1}{2}}\|^2, \\ (\mu_e (u^{n+\frac{1}{2}} - \widehat{u}_h^{n+\frac{1}{2}}) \cdot \nabla \overline{\xi}_e^{n+\frac{1}{2}}, \overline{\xi}_e^{n+\frac{1}{2}}) & \end{aligned}$$

$$\begin{aligned} &\leq \frac{1}{24} D_{e,*} \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M D_{e,*}^{-1} \|u^{n+\frac{1}{2}} - \hat{u}_h^{n+\frac{1}{2}}\|_\infty^2 \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \\ &\leq \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2. \end{aligned}$$

所以

$$\begin{aligned} (\mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}, \bar{\xi}_e^{n+\frac{1}{2}}) &\leq \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2, \\ (\nabla \cdot (D_e \nabla \bar{\xi}_e^{n+\frac{1}{2}}), \delta_e \mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}) &\leq \frac{1}{8} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2. \end{aligned}$$

综合以上各式得:

$$\begin{aligned} B_n(\bar{\xi}_e^{n+\frac{1}{2}}, \bar{\xi}_e^{n+\frac{1}{2}}) &\geq \frac{1}{2\Delta t} (\|\xi_e^{n+1}\|^2 - \|\xi_e^n\|^2) + \frac{\delta_e}{2} \|\mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + \frac{5}{6} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 \\ &\quad - \left[\frac{\delta_e}{2} \|\bar{d}_t \xi_e^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \right]. \end{aligned} \quad (5.16)$$

再估计右端项. 注意到 $2\delta_e \mu_e^* u^* C_0 h^{-1} \leq \frac{1}{24}$, 我们有估计:

$$\begin{aligned} (\bar{d}_t \bar{\eta}_e^{n+\frac{1}{2}}, \bar{\xi}_e^{n+\frac{1}{2}} - \delta_e \mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}) &\leq M(\|d_t \bar{\eta}_e^{n+\frac{1}{2}}\|^2 + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2), \\ (\mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\eta}_e^{n+\frac{1}{2}}, \delta_e \mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}) &\leq \frac{1}{24} \delta_e \|\mu_e u_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M \delta_e \|\nabla \bar{\eta}_e^{n+\frac{1}{2}}\|^2, \\ (\mu_e u^{n+\frac{1}{2}} \cdot \nabla \bar{\eta}_e^{n+\frac{1}{2}}, \bar{\xi}_e^{n+\frac{1}{2}}) \\ &= -(\bar{\eta}_e^{n+\frac{1}{2}}, \nabla \cdot (\mu_e u^{n+\frac{1}{2}} \bar{\xi}_e^{n+\frac{1}{2}}) - (\bar{\eta}_e^{n+\frac{1}{2}}, \mu_e u^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}) \\ &\leq M\{\|\bar{\eta}_e^{n+\frac{1}{2}}\|^2 + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2\} + \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M D_{e,*}^{-1} \|\bar{\eta}_e^{n+\frac{1}{2}}\|^2, \\ (\mu_e (\hat{u}_h^{n+\frac{1}{2}} - u^{n+\frac{1}{2}}) \nabla \bar{\eta}_e^{n+\frac{1}{2}}, \bar{\xi}_e^{n+\frac{1}{2}}) &\leq M(\tilde{K})(h^{2r+1} + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2), \end{aligned}$$

于是

$$\begin{aligned} (\mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \bar{\eta}_e^{n+\frac{1}{2}}, \bar{\xi}_e^{n+\frac{1}{2}}) &\leq \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M(\tilde{K})(h^{2r+1} + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2), \\ (D_e \nabla \bar{\eta}_e^{n+\frac{1}{2}}, \nabla \bar{\xi}_e^{n+\frac{1}{2}}) &\leq \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M D_{e,*} \|\nabla \bar{\eta}_e^{n+\frac{1}{2}}\|^2. \end{aligned}$$

类似于 (3.6) 式, 我们有

$$\begin{aligned} &(\nabla \cdot (D_e \nabla \bar{\eta}_e^{n+\frac{1}{2}}), \delta_e \mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}) \\ &\leq \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M D_{e,*} \left(\|\nabla \bar{\eta}_e^{n+\frac{1}{2}}\|^2 + \delta_e \sum_{\tau_k \in T_h} \int_{\partial \tau_k} |\nabla \bar{\eta}_e^{n+\frac{1}{2}}|^2 ds \right). \end{aligned}$$

综合以上各式, 再注意到 (4.5) 和 (4.6), 我们有估计

$$\begin{aligned} B_n(\bar{\eta}_e^{n+\frac{1}{2}}, \bar{\xi}_e^{n+\frac{1}{2}}) &\leq \frac{1}{24} \delta_e \|\mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + \frac{1}{8} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 \\ &\quad + M(\tilde{K}) (\|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 + D_{e,*} h^{2r} + h^{2r+1}), \end{aligned} \quad (5.17)$$

$$|Q_1| \leq M \left((\Delta t)^3 \left\| \frac{\partial^3 e}{\partial t^3} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \right), \tag{5.18}$$

$$\begin{aligned} |Q_2| &\leq M \left(\|\hat{u}_h^{n+\frac{1}{2}} - u^{n+\frac{1}{2}}\|^2 + \|\nabla \bar{e}^{n+\frac{1}{2}} - \nabla e^{n+\frac{1}{2}}\|^2 + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \right) \\ &\leq M \left(h^{2r+2} + (\Delta t)^3 \left(\left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \nabla \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right) \right) \\ &\quad + M \left(\|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\xi_e^{n+1}\|^2 \right), \end{aligned} \tag{5.19}$$

$$|Q_3| \leq M \left((\Delta t)^3 \left\| \nabla \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \right), \tag{5.20}$$

$$|Q_4| \leq M \left((\Delta t)^3 \left(\left\| \nabla \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \Delta \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right) + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \right), \tag{5.21}$$

$$\begin{aligned} |Q_5| + |Q_6| &\leq M \left(\|\hat{e}_h^{n+\frac{1}{2}} - e^{n+\frac{1}{2}}\|^2 + \|\hat{p}_h^{n+\frac{1}{2}} - p^{n+\frac{1}{2}}\|^2 + \|\hat{u}_h^{n+\frac{1}{2}} - u^{n+\frac{1}{2}}\|^2 + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \right) \\ &\leq M \left\{ h^{2r+2} + (\Delta t)^3 \left(\left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right) \right. \\ &\quad \left. + \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right) + \|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\xi_e^{n+1}\|^2 \}. \end{aligned} \tag{5.22}$$

由 R 的 Lipschitz 连续性, 我们得:

$$\begin{aligned} |Q_7| &\leq M \left(\|\hat{e}_h^{n+\frac{1}{2}} - e^{n+\frac{1}{2}}\|^2 + \|\hat{p}_h^{n+\frac{1}{2}} - p^{n+\frac{1}{2}}\|^2 + \|\hat{T}_h^{n+\frac{1}{2}} - T^{n+\frac{1}{2}}\|^2 + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 \right) \\ &\leq M \left\{ h^{2r+2} + (\Delta t)^3 \left(\left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right) \right. \\ &\quad \left. + \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right) + \|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 \\ &\quad \left. + \|\xi_e^{n+1}\|^2 + \|\xi_T^{n-1}\|^2 + \|\xi_T^n\|^2 \right\}. \end{aligned} \tag{5.23}$$

如果 $n = 0$, 注意到 (5.13) 和 (5.14), $Q_1 \sim Q_7$ 右端的上标 $n-1$ 改为 0. 结合 (5.16)–(5.23) 得:

$$\begin{aligned} &\frac{1}{2\Delta t} (\|\xi_e^{n+1}\|^2 - \|\xi_e^n\|^2) + \frac{11}{24} \delta_e \|\mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + \frac{17}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 \\ &\leq \frac{\delta_e}{2} \|\bar{d}_t \xi_e^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \left\{ D_{e,*} h^{2r} + h^{2r+1} + (\Delta t)^{-1} h^{2r+2} \left\| \frac{\partial e}{\partial t} \right\|_{L^2(t^n, t^{n+1}; H^{r+1})}^2 \right. \\ &\quad + (\Delta t)^3 \left(\left\| \nabla \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \Delta \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right) \\ &\quad + \left\| \frac{\partial^3 e}{\partial t^3} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 P}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \\ &\quad + \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \left. \right) + \|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 \\ &\quad + \|\xi_e^{n+1}\|^2 + \|\xi_T^{n-1}\|^2 + \|\xi_T^n\|^2 \}. \end{aligned} \tag{5.24}$$

与此对应的还有空穴浓度的估计:

$$\frac{1}{2\Delta t} (\|\xi_p^{n+1}\|^2 - \|\xi_p^n\|^2) + \frac{11}{24} \delta_e \|\mu_e \hat{u}_h^{n+\frac{1}{2}} \cdot \nabla \bar{\xi}_p^{n+\frac{1}{2}}\|^2 + \frac{17}{24} D_{p,*} \|\nabla \bar{\xi}_p^{n+\frac{1}{2}}\|^2$$

$$\begin{aligned}
&\leq \frac{\delta_e}{2} \|\bar{d}_t \xi_p^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \left\{ D_{p,*} h^{2r} + h^{2r+1} + (\Delta t)^{-1} h^{2r+2} \left\| \frac{\partial p}{\partial t} \right\|_{L^2(t^n, t^{n+1}; H^{r+1})}^2 \right. \\
&\quad + (\Delta t)^3 \left(\left\| \nabla \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \Delta \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right. \\
&\quad + \left\| \frac{\partial^3 p}{\partial t^3} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \\
&\quad + \left. \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right) + \|\xi_p^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_p^n\|^2 + \|\xi_e^n\|^2 \\
&\quad + \left. \|\xi_p^{n+1}\|^2 + \|\xi_T^{n-1}\|^2 + \|\xi_T^n\|^2 \right\}. \tag{5.25}
\end{aligned}$$

估计 $\|\bar{d}_t \xi_e^{n+\frac{1}{2}}\|$. 在误差方程 (5.10) 中, 令 $v_h = \bar{d}_t \xi_e^{n+\frac{1}{2}}$. 完全类似于 (5.11)–(5.24), 成立

$$\begin{aligned}
&B_n(\bar{\xi}_e^{n+\frac{1}{2}}, d_t \xi_e^{n+\frac{1}{2}}) \geq \frac{5}{6} \|\bar{d}_t \xi_e^{n+\frac{1}{2}}\|^2 - (\mu_e^{*2} u^{*2} + 8q_e^2 D_{e,*}^2 C_0^2 h^{-2}) \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2, \\
&B_n(\bar{\eta}_e^{n+\frac{1}{2}}, d_t \xi_e^{n+\frac{1}{2}}) \\
&\leq \varepsilon \|d_t \xi_e^{n+\frac{1}{2}}\|^2 + M_\varepsilon \left\{ \delta_e^{-1} (h^{2r+1} + D_{e,*} h^{2r}) + (\Delta t)^{-1} h^{2r+2} \left\| \frac{\partial e}{\partial t} \right\|_{L^2(t^n, t^{n+1}; H^{r+1})}^2 \right\}.
\end{aligned}$$

相应的 $Q_1 \sim Q_7$ 项均为常规估计. 取 ε 充分小可得:

$$\begin{aligned}
&\frac{2}{3} \|d_t \xi_e^{n+\frac{1}{2}}\|^2 \\
&\leq (\mu_e^{*2} u^{*2} + 8q_e^2 D_{e,*}^2 C_0^2 h^{-2}) \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \left\{ \delta_e^{-1} (D_{e,*} h^{2r} + h^{2r+1}) \right. \\
&\quad + (\Delta t)^{-1} h^{2r+2} \left\| \frac{\partial e}{\partial t} \right\|_{L^2(t^n, t^{n+1}; H^{r+1})}^2 + (\Delta t)^3 \left(\left\| \nabla \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right. \\
&\quad + \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \Delta \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^3 e}{\partial t^3} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \\
&\quad + \left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \\
&\quad + \left. \|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\xi_e^{n+1}\|^2 + \|\xi_T^{n-1}\|^2 + \|\xi_T^n\|^2 \right\}. \tag{5.26}
\end{aligned}$$

对于空穴浓度 $\|\bar{d}_t \xi_p^{n+\frac{1}{2}}\|$ 有类似的估计:

$$\begin{aligned}
&\frac{2}{3} \|\bar{d}_t \xi_p^{n+\frac{1}{2}}\|^2 \\
&\leq (\mu_e^{*2} u^{*2} + 8q_p^2 D_{p,*}^2 C_0^2 h^{-2}) \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \left\{ \delta_p^{-1} (D_{p,*} h^{2r} + h^{2r+1}) \right. \\
&\quad + (\Delta t)^{-1} h^{2r+2} \left\| \frac{\partial p}{\partial t} \right\|_{L^2(t^n, t^{n+1}; H^{r+1})}^2 + (\Delta t)^3 \left(\left\| \nabla \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right. \\
&\quad + \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \Delta \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^3 p}{\partial t^3} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \\
&\quad + \left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \\
&\quad + \left. \|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\xi_p^{n+1}\|^2 + \|\xi_T^{n-1}\|^2 + \|\xi_T^n\|^2 \right\}. \tag{5.27}
\end{aligned}$$

下面估计温度方程的误差. 易得误差方程: 对任何 $v_h \in S_h$, 成立

$$\begin{aligned}
 & (\rho \bar{d}_t \xi_T^{n+\frac{1}{2}}, v_h) + (\nabla \bar{\xi}_T^{n+\frac{1}{2}}, \nabla v_h) \\
 &= (\rho(\bar{d}_t \eta_T^{n+\frac{1}{2}} + T_t^{n+\frac{1}{2}} - d_t T^{n+\frac{1}{2}}), v_h) + (\nabla(T^{n+\frac{1}{2}} - \bar{T}^{n+\frac{1}{2}}), \nabla v_h) \\
 &+ (\hat{u}_h^{n+\frac{1}{2}}(D_e \nabla \bar{e}_h^{n+\frac{1}{2}} - D_p \nabla \bar{p}_h^{n+\frac{1}{2}}) - u^{n+\frac{1}{2}}(D_e \nabla e^{n+\frac{1}{2}} - D_p \nabla p^{n+\frac{1}{2}}), v_h) \\
 &+ (\hat{u}_h^{n+\frac{1}{2}} \cdot \hat{u}_h^{n+\frac{1}{2}}(\mu_p \bar{p}_h^{n+\frac{1}{2}} - \mu_e \bar{e}_h^{n+\frac{1}{2}}) \\
 &- u^{n+\frac{1}{2}} \cdot u^{n+\frac{1}{2}}(\mu_p p^{n+\frac{1}{2}} - \mu_e e^{n+\frac{1}{2}}), v_h). \tag{5.28}
 \end{aligned}$$

在 (5.28) 中, 令 $v_h = \bar{\xi}_T^{n+\frac{1}{2}}$, 右端项依次记为 $W_1 \sim W_4$. 逐项估计得:

$$(\rho \bar{d}_t \xi_T^{n+\frac{1}{2}}, \bar{\xi}_T^{n+\frac{1}{2}}) + (\nabla \bar{\xi}_T^{n+\frac{1}{2}}, \nabla \bar{\xi}_T^{n+\frac{1}{2}}) \geq \frac{1}{2\Delta t} \{ \|\rho \xi_T^{n+1}\|^2 - \|\rho \xi_T^n\|^2 \} + \|\nabla \bar{\xi}_T^{n+\frac{1}{2}}\|^2, \tag{5.29}$$

$$W_1 \leq M \left((\Delta t)^{-1} h^{2r+2} \left\| \frac{\partial T}{\partial t} \right\|_{L^2(t^n, t^{n+1}; H^{r+1})}^2 + (\Delta t)^3 \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \|\bar{\xi}_T^{n+\frac{1}{2}}\|^2 \right), \tag{5.30}$$

$$W_2 \leq \varepsilon \|\nabla \bar{\xi}_T^{n+\frac{1}{2}}\|^2 + M_\varepsilon (\Delta t)^3 \left\| \frac{\partial^2 T}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2, \tag{5.31}$$

$$\begin{aligned}
 W_3 \leq & \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + \frac{1}{24} D_{p,*} \|\nabla \bar{\xi}_p^{n+\frac{1}{2}}\|^2 + M(\tilde{K})(D_{e,*} h^{2r} + D_{p,*} h^{2r} + h^{2r+2}) \\
 & + M(\tilde{K})(\Delta t)^3 \left(\left\| \nabla \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \nabla \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right. \\
 & \left. + \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 \right) + M(\tilde{K})(\|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 \\
 & + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\xi_T^n\|^2 + \|\xi_T^{n+1}\|^2). \tag{5.32}
 \end{aligned}$$

如果 $n = 0$, 右端上标 $n - 1$ 变为 0.

$$\begin{aligned}
 W_4 \leq & M(h^{2r+2} + \|\bar{\xi}_e^{n+\frac{1}{2}}\|^2 + \|\bar{\xi}_p^{n+\frac{1}{2}}\|^2 + \|\bar{\xi}_T^{n+\frac{1}{2}}\|^2) + M \left(\|\hat{u}_h^{n+\frac{1}{2}} - u^{n+\frac{1}{2}}\|^2 \right. \\
 & \left. + (\Delta t)^3 \left(\left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right) \right). \tag{5.33}
 \end{aligned}$$

取 ε 充分小, 结合 (5.28)-(5.33) 得:

$$\begin{aligned}
 & \frac{1}{2\Delta t} \{ \|\rho \xi_T^{n+1}\|^2 - \|\rho \xi_T^n\|^2 \} + \frac{1}{2} \|\nabla \bar{\xi}_T^{n+\frac{1}{2}}\|^2 \\
 \leq & \frac{1}{24} D_{e,*} \|\nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + \frac{1}{24} D_{p,*} \|\nabla \bar{\xi}_p^{n+\frac{1}{2}}\|^2 + M(\tilde{K}) \{ D_{e,*} h^{2r} + D_{p,*} h^{2r} + h^{2r+1} \\
 & + (\Delta t)^{-1} h^{2r+2} \left\| \frac{\partial T}{\partial t} \right\|_{L^2(t^n, t^{n+1}; H^{r+1})}^2 + (\Delta t)^3 \left(\left\| \nabla \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right. \\
 & \left. + \left\| \nabla \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 u}{\partial t^2} \right\|_{L^2(t^{n-1}, t^{n+1}; L^2)}^2 + \left\| \frac{\partial^2 p}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right. \\
 & \left. + \left\| \frac{\partial^2 e}{\partial t^2} \right\|_{L^2(t^n, t^{n+1}; L^2)}^2 \right) + \|\xi_e^{n-1}\|^2 + \|\xi_p^{n-1}\|^2 + \|\xi_e^n\|^2 + \|\xi_p^n\|^2 \\
 & + \|\xi_T^{n-1}\|^2 + \|\xi_T^n\|^2 + \|\xi_T^{n+1}\|^2 \}. \tag{5.34}
 \end{aligned}$$

令 (5.24) + (5.25) + $\delta_e(5.26)$ + $\delta_p(5.27)$ + (5.34), 两边乘 $2\Delta t$, 然后关于 n 求和. 注意到 $\xi_s^0 = 0$, $s = e, p, T$, 利用离散 Gronwall 引理, 我们有误差估计:

$$\begin{aligned} & \|\xi_e^n\|^2 + \|\xi_p^n\|^2 + \|\xi_T^n\|^2 + \sum_{j=0}^{n-1} [\delta_e \|\mu_e \hat{u}_h^{j-\frac{1}{2}} \cdot \nabla \bar{\xi}_e^{n+\frac{1}{2}}\|^2 + \delta_p \|\mu_p \hat{u}_h^{j-\frac{1}{2}} \cdot \nabla \bar{\xi}_p^{j+\frac{1}{2}}\|^2] \Delta t \\ & + \sum_{j=0}^{n-1} [D_{e,*} \|\nabla \bar{\xi}_e^{j+\frac{1}{2}}\|^2 + D_{p,*} \|\nabla \bar{\xi}_p^{j+\frac{1}{2}}\|^2 + \|\nabla \bar{\xi}_T^{j+\frac{1}{2}}\|^2] \\ & + \sum_{j=0}^{n-1} [\delta_e \|\bar{d}_t \xi_e^{j+\frac{1}{2}}\|^2 + \delta_p \|\bar{d}_t \xi_p^{j+\frac{1}{2}}\|^2] \Delta t \\ & \leq M(\tilde{K}) \{D_{e,*} h^{2r} + D_{p,*} h^{2r} + h^{2r+1} + (\Delta t)^4\}. \end{aligned} \quad (5.35)$$

下面验证归纳假定 (5.15). 当 $n = 0$ 时,

$$\begin{aligned} \|\hat{u}_h^{\frac{1}{2}} - u^{\frac{1}{2}}\|_\infty & \leq \|u_h^0 - u_0\|_\infty + \frac{\Delta t}{2} \|u_{ht}^0 - u_t^0\|_\infty + \left\| \int_0^{t^{\frac{1}{2}}} (t^{\frac{1}{2}} - t) \frac{\partial^2 u}{\partial t^2} dt \right\|_\infty \\ & \leq Mh^r + M\Delta t(h^r + h^{-\frac{3}{2}}h^r) + \Delta t \left\| \frac{\partial^2 u}{\partial t^2} \right\|_\infty \leq Mh^{\frac{1}{2}}, \end{aligned} \quad (5.36)$$

其中 M 与 $1/D_{e,*}$ 和 $1/D_{p,*}$ 无关. 假定 (5.15a) 对 $0 \leq j \leq n-1$ 成立, 则由 (5.35) 式

$$\begin{aligned} & \|u_h^{n+\frac{1}{2}} - u^{n+\frac{1}{2}}\|_\infty \\ & \leq \frac{3}{2} \|u_h^n - u^n\|_\infty + \frac{1}{2} \|u_h^{n-1} - u^{n-1}\|_\infty + 2\Delta t \left\| \frac{\partial^2 u}{\partial t^2} \right\|_\infty \\ & \leq M(h^r + \Delta t) + M(\tilde{K})h^{-\frac{3}{2}} [h^{r+1} + \|\xi_e^{n-1}\| + \|\xi_p^{n-1}\| + \|\xi_e^n\| + \|\xi_p^n\|] \\ & \leq Mh^{\frac{1}{2}}. \end{aligned} \quad (5.37)$$

这里 M 不依赖于 $1/D_{e,*}$ 和 $1/D_{p,*}$. 当 h 充分小时, $\|\hat{u}_h^{n+\frac{1}{2}}\|_\infty \leq 2K^*$ 成立.

再验证 $\|\hat{s}_n^{n+\frac{1}{2}}\|_\infty \leq 3s^*$, $s = e, p$. 当 $n = 0$ 时,

$$\begin{aligned} \|s_h^{\frac{1}{2}}\|_\infty & \leq s^* + \frac{\Delta t}{2} \|s_{ht}^0\|_\infty \leq s^* + \frac{\Delta t}{2} \|s_t^0\|_\infty + \frac{\Delta t}{2} \|s_t^0 - s_{ht}^0\|_\infty \\ & \leq s^* + \frac{\Delta t}{2} \|s_t^0\|_\infty + \frac{\Delta t}{2} \|u^0 - u_h^0\|_\infty \leq s^* + Mh^{1+\sigma} \leq 2K^*. \end{aligned} \quad (5.38)$$

设 (5.15b) 对 $0 \leq j \leq n-1$ 成立, 则由 (5.34), 注意到 $r \geq 2$,

$$\begin{aligned} \|\hat{s}_h^{n+\frac{1}{2}}\|_\infty & \leq \|\hat{s}^{n+\frac{1}{2}}\|_\infty + \|\hat{\eta}_s^{n+\frac{1}{2}}\|_\infty + \|\hat{\xi}_s^{n+\frac{1}{2}}\|_\infty \\ & \leq 2s^* + M(h^{r-\frac{1}{2}} + h^{-\frac{3}{2}}(h^{r+1} + (\sqrt{D_{e,*}} + \sqrt{D_{p,*}})h^r + (\Delta t)^2)). \end{aligned} \quad (5.39)$$

因此, 当 h 适当小时, 归纳假定 (5.15) 成立. 再由 (5.34), 结合投影误差 (4.3), (4.5) 和 (4.8) 即得 (5.4). 定理 2 证毕.

致谢 作者感谢审稿人提出的修改意见.

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C-N DIFFERENCE STREAMLINE DIFFUSION METHOD FOR THREE-DIMENSIONAL SEMICONDUCTOR PROBLEM WITH HEAT-CONDUCTION AND NUMERICAL ANALYSIS

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Abstract In this article, we study the numerical method for simulation of three-dimensional semiconductor problem with heat-conduction. Considering different types of partial differential equations arising from the model for the transient behavior of a semiconductor device, we present different finite element scheme respectively. Especially, we use Crank-Nicolson difference streamline diffusion method to treat convection-diffusion equations of the concentrations of electron and hole in the model. The numerical stability is improved by difference streamline diffusion method. An error estimate in L^2 norm with quasi-optimal accuracy in space and second order accuracy in time is derived.

Key words Three-dimensional heat conduction, semiconductor, C-N scheme, difference streamline diffusion method, error estimate