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for Contaminant Transport with
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Abstract

A procedure based on combining the method of characteristics with a Galerkin finite element method is analyzed for approximating reactive transport in groundwater. In particular, we consider equations modeling contaminant transport with nonlinear, non-equilibrium adsorption reactions. This phenomenon gives rise to non-Lipschitz but monotone nonlinearities which complicate the analysis. A physical and mathematical description of the problem under consideration is given, then the numerical method is described and *a priori* error estimates are derived.

Keywords: method of characteristics, Galerkin finite elements, contaminant transport

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1 Introduction

In this paper, we describe a characteristic-Galerkin finite element method (CGFEM) for modeling contaminant transport with nonlinear, non-equilibrium adsorption kinetics. The CGFEM, also known as the modified method of characteristics, Lagrange-Galerkin, or Euler-Lagrange method, has been used extensively in the modeling of linear and nonlinear flows; see, for example, [10, 14, 15, 16]. The method was first analyzed in [4] for advective flow problems in one space dimension, and improvements and extensions of these estimates were derived in [5]. These estimates were proved primarily for linear problems; however, certain types of smooth nonlinearities were also considered.

Here we consider the application of the CGFEM to a nonlinear system of equations which arises in contaminant transport, and derive an *a priori* error estimate. The primary difficulty in these equations is the presence of possibly non-Lipschitz nonlinearities, which require special treatment in the analysis. The presence of such nonlinearities also reduces the regularity of the solution; thus, the expected rates of convergence are possibly suboptimal when approximating by piecewise polynomials.

Error estimates for a Galerkin finite element procedure for solving these types of equations have recently been derived in [1]. The approach given there involves approximating the solution to a regularized problem, obtained by replacing the non-Lipschitz function ϕ (given by (3.9) below) with a Lipschitz approximation ϕ_ϵ , and allowing ϵ to approach zero. The estimates obtained for this procedure in the norm $L^\infty(0, T; L^2(\Omega))$ appear to give the same or a slightly improved rate of convergence

than that derived below for the CGFEM, depending on the choice of ϵ . However, the authors are able to obtain a better rate of convergence in the $L^2(0, T; L^2(\Omega))$ norm. Numerical comparisons of the two approaches remains to be done. We note that our approach is better suited for convection-dominated transport.

In the next section, we give some basic notation. In Sections 3 and 4, the physical problem is described, and existence and uniqueness of weak solutions, and regularity of solutions are discussed. In Section 5, we describe the application of the CGFEM method, and in Section 6, the method is analyzed, assuming optimal regularity of the solution.

2 Notation

For Y a measurable space or space-time domain, let $L^p(Y)$, $1 \leq p \leq \infty$, denote the standard Banach space on Y , with norm $\|\cdot\|_{L^p(Y)}$. For Ω a bounded spatial domain in \mathbb{R}^d , $1 \leq d \leq 3$, denote by $W_2^k(\Omega)$ the standard Sobolev space on Ω with norm $\|\cdot\|_k$. We denote the $L^2(\Omega)$ norm by $\|\cdot\|$.

Let $[\alpha, \beta] \subset [0, T]$ denote a time interval, where $T > 0$ is a fixed constant, and let $X = X(\Omega)$ denote a normed space. Denote by $\|\cdot\|_{L^p(\alpha, \beta; X)}$ the norm of X -valued functions f with the map $t \rightarrow \|f(\cdot, t)\|_X$ belonging to $L^p(\alpha, \beta)$.

Letting $Q_T = \Omega \times (0, T]$, we denote by $V_2^{1,0}(Q_T)$ the Banach space consisting of elements having a finite norm

$$|u|_{Q_T} = \|u\|_{L^\infty(0, T; L^2(\Omega))} + \|\nabla u\|_{L^2(0, T; L^2(\Omega))}.$$

We denote by $W_2^{1,1}(Q_T)$ the Hilbert space with scalar product

$$(u, v)_{W_2^{1,1}(Q_T)} = \int_{Q_T} (uv + \nabla u \cdot \nabla v + u_t v_t) dx dt.$$

For $\phi : [0, \infty) \rightarrow [0, \infty)$, the notation $\phi \in C^p([0, \infty))$, $p \in (0, 1)$ means ϕ is Hölder continuous in its argument with exponent p . We denote by $C^{\alpha, \beta}(Q_T)$, where α and β are positive numbers, the standard Hölder space defined on Q_T [12]. Here α represents smoothness in space and β represents smoothness in time.

3 Statement of the Problem

When chemical species are dissolved in groundwater they may undergo adsorption or exchange processes on the surface of the porous skeleton. Knowledge about the influence of these chemical processes on the transport of the solutes when the groundwater is moving is of fundamental importance to understand, for instance, how pollutants spread in space and time through the soil.

Below we present the mathematical formulation for a one-species system in which the chemicals undergo non-equilibrium adsorption reactions. Certain types of two-species systems of binary ion exchange can also be put into this framework. In particular this is the case when a conservation property allows for the reduction to a one-species system. In [8], details of this reduction are given, as well as a fundamental discussion of adsorption processes in porous media and related references.

The domain Ω is occupied by a porous material through which an incompressible fluid, say water, flows. The related specific discharge $\bar{q}(m/s)$, with components $q_i, i =$

$1, \dots, d$ and length $|\bar{q}|$, satisfies the equation

$$\frac{\partial \theta}{\partial t} + \nabla \cdot \bar{q} = 0, \quad (3.1)$$

which expresses conservation of fluid volume. In this equation, θ (dimensionless) denotes the water content.

In what follows we shall consider θ and \bar{q} as given quantities which are determined independently of the concentration of the dissolved chemicals. Thus, we implicitly assume here that concentrations occur only at tracer levels and hence do not influence the flow.

Let $c(\text{mol}/m^3)$ denote the concentration of adsorbate in solution and $A(\text{mol}/\text{kg porous medium})$ the adsorbed concentration. Conservation for the chemical species gives the equation

$$\frac{\partial}{\partial t} (\theta c + \rho A) + \nabla \cdot (\bar{q} c - \theta D \nabla c) = 0, \quad (3.2)$$

in which $\rho = \rho(x)$ ($\text{kg porous medium}/m^3$) denotes the density of the porous medium (bulk density), and $D(m^2/s)$ the hydrodynamic dispersion matrix which incorporates the effects of molecular diffusion and mechanical (velocity-dependent) dispersion. In most transport models for porous media D takes the form, e.g. see [2]

$$\theta D_{ij} = \left\{ \theta D_{\text{mol}} + \alpha_T |\bar{q}| \right\} \delta_{ij} + (\alpha_L - \alpha_T) \frac{q_i q_j}{|\bar{q}|} \quad i, j = 1, \dots, d, \quad (3.3)$$

where $D_{\text{mol}}(m^2/s)$ is the molecular diffusivity of the adsorbate in the fluid (incorporating the tortuosity effect) and $\alpha_T(m)$ and $\alpha_L(m)$ are the transverse and longitudinal dispersion lengths, respectively.

Next we turn to the adsorption process. In this paper we assume that the reactions

are relatively slow compared to the flow of the fluid. This makes it necessary to consider non-equilibrium adsorption. In addition, the adsorbent surface of the grains may be heterogeneous. Consider a subdivision of a representative grain surface (i.e. rescaled grain surface, e.g. the unit sphere) into m chemically different collections of adsorption sites corresponding to $i \in \{1, \dots, m\}$; let λ_i be their relative size at the representative grain surface and s_i the corresponding adsorbed concentration. Then

$$\sum_{i=1}^m \lambda_i = 1 \quad (\lambda_i > 0), \quad (3.4)$$

and

$$A = \sum_{i=1}^m \lambda_i s_i. \quad (3.5)$$

Each component s_i is related to the dissolved concentration c through an adsorption reaction which is described by the first order equation

$$\frac{\partial s_i}{\partial t} = k f_i(c, s_i) \quad \text{with} \quad i \in \{1, \dots, m\}. \quad (3.6)$$

In these equations $k > 0$ ($1/s$) is the rate constant, and f_i is the rate function describing the adsorption reactions at sites i . In principle, k and $\lambda_1, \dots, \lambda_m$ could be spatially dependent; however, for simplicity, we assume they are constant in space and time and k is independent of i . For the rate function in (3.6) we use the explicit form

$$f_i(c, s_i) = \phi_i(c) - s_i, \quad i \in \{1, \dots, m\}, \quad (3.7)$$

which, in a heuristic approach, is widely used in contaminant transport models, e.g. see [3]. The functions ϕ_i in (3.7) are called the adsorption isotherms. They are the

adsorbed concentrations in the equilibrium, i.e. fast reaction case, as $k \rightarrow \infty$. Typical examples are the Langmuir isotherm

$$\phi(c) = \frac{K_1 c}{1 + K_2 c}, \quad K_1, K_2 > 0, \quad (3.8)$$

and the Freundlich isotherm

$$\phi(c) = K_3 c^p, \quad K_3 > 0, p > 0. \quad (3.9)$$

In the last example one usually takes $p \in (0, 1]$. For $p < 1$, the nonlinearities are not Lipschitz continuous up to $c = 0$. This results in the finite speed of propagation property for the concentration c as $c \downarrow 0$, and thus gives rise to a free boundary as the boundary of the support of c .

Thus, together with the transport equation (3.2), with A given by (3.5), we have to solve for the m -O.D.E.'s

$$\frac{\partial s_i}{\partial t} = k(\phi_i(c) - s_i) \quad \text{with} \quad i \in \{1, \dots, m\}. \quad (3.10)$$

We consider (3.1), (3.2), (3.5) and (3.10) in the cylinder $Q_T = \Omega \times (0, T]$.

For all unknowns c and s_i we need to specify initial conditions. Thus

$$c(\cdot, 0) = c_0 \quad \text{and} \quad s_i(\cdot, 0) = s_{0i} \quad \text{in } \Omega, \quad (3.11)$$

for $i \in \{1, \dots, m\}$. In addition we prescribe for c conditions along the boundary $\mathcal{S} = \partial\Omega$ of Ω . Letting $\alpha = -\bar{n} \cdot \bar{q}$, we distinguish an inflow boundary S_1 where $\alpha \geq 0$ and an outflow/no flow boundary S_2 where $\alpha \leq 0$. Here $S_1 \cup S_2 = \mathcal{S}$ and \bar{n} denotes the outer unit normal. Then we impose

$$(\theta D\nabla c - \bar{q}c) \cdot \bar{n} = F \quad \text{on} \quad S_{1T} = S_1 \times (0, T], \quad (3.12)$$

$$(\theta D \nabla c) \cdot \bar{n} = 0 \quad \text{on} \quad S_{2T} = S_2 \times (0, T]. \quad (3.13)$$

In (3.12), the function $F = F(x, t)$, with $(x, t) \in S_{1T}$, denotes the flux of solute entering the flow domain across S_1 at time $t > 0$.

Equations (3.1)–(3.13) define the Contaminant Transport Model, which we shall refer to as Problem CTM. In defining a weak solution or a weak formulation for Problem CTM we follow the usual definition for linear problems, e.g. see [12] and [11]. In particular we use the space $V_2^{1,0}(Q_T)$. Then we have the following definition.

Definition 3.1 *The functions $c, s_i : \bar{Q}_T \rightarrow [0, \infty)$ for $i \in \{1, \dots, m\}$ form a weak solution of Problem CTM if the following holds:*

- (i) $c \in V_2^{1,0}(Q_T)$, $\phi_i(c) \in L^2(Q_T)$ for $i \in \{1, \dots, m\}$;
- (ii) $s_i, \frac{\partial s_i}{\partial t} \in L^2(Q_T)$ for $i \in \{1, \dots, m\}$;
- (iii)
$$\begin{aligned}
& - \int_{\Omega} (\theta c \eta)(\cdot, 0) - \int_{Q_T} \theta c \frac{\partial \eta}{\partial t} + \int_{Q_T} \rho \left(\sum_{i=1}^m \lambda_i \frac{\partial s_i}{\partial t} \right) \eta \\
& + \int_{Q_T} (\theta D \nabla c - \bar{q} c) \cdot \nabla \eta = \int_{S_{1T}} F \eta + \int_{S_{2T}} \alpha c \eta, \quad (3.14)
\end{aligned}$$
for all $\eta \in W_2^{1,1}(Q_T)$ which vanish at $t = T$;
- (iv) $\frac{\partial s_i}{\partial t} = k \{\phi_i(c) - s_i\}$, $i \in \{1, \dots, m\}$, $(x, t) \in Q_T$;
- (v) $c(\cdot, 0) = c_0$ and $s_i(\cdot, 0) = s_{0i}$, $i \in \{1, \dots, m\}$, $(x, t) \in Q_T$.

Throughout this paper we take \mathcal{S} to be piecewise smooth. With respect to the coefficients and functions appearing in Definition 3.1 we shall assume that the following structural and regularity conditions are satisfied; see also [6] and [11].

(H1a) For each $i \in \{1, \dots, m\}$ the isotherms $\phi_i : [0, \infty) \rightarrow [0, \infty)$ are nondecreasing;

(H1b) There are constants $\nu, \mu > 0$ such that for $\xi \in \mathbb{R}^d$, $(x, t) \in Q_T$,

$$\nu |\xi|^2 \leq \xi^T (\theta D)(x, t) \xi \leq \mu |\xi|^2 ,$$

the D_{ij} are measurable in Q_T , $\partial_t D_{ij} \in L^\infty(Q_T)$ for $i, j = 1, \dots, d$,

θD is symmetric;

(H1c) There exists $\theta_0 > 0$ such that

$$\theta(x, t) \geq \theta_0 \quad \text{for } (x, t) \in Q_T ,$$

$$\theta, \partial_t \theta \in L^\infty(Q_T);$$

(H1d) $q_i \in L^\infty(Q_T)$ for $i = 1, \dots, d$, $\nabla \cdot \bar{q} \in L^\infty(Q_T)$, $\bar{q} \cdot \bar{n}$ exists in the sense of trace and $\bar{q} \cdot \bar{n} \in L^\infty(S_T)$, θ and \bar{q} satisfy equation (3.1);

(H1e) $F \in L^\infty(S_{1T})$, $c_0, s_{0i} \geq 0$ and $c_0, s_{0i} \in L^2(\Omega)$ for $i \in \{1, \dots, m\}$;

(H1f) $\rho \in L^\infty(\Omega)$, $\rho \geq \rho_* > 0$, for some positive constant ρ_* .

4 Some Analytical Observations

Weak solutions of Problem CTM, in the sense of Definition 3.1, were studied in [6] and [11]. The main, and nonstandard, difficulty for this problem lies in the fact that one of the isotherms ϕ_i may be non-smooth at $c = 0$. This happens for instance when it is of Freundlich type, see (3.9). Then a situation may occur where the set $\{c > 0\}$ spreads at finite speed through the flow domain Ω . A free boundary or interface arises

as the boundary of the support of c , i.e. $\partial\{c > 0\}$. Across the free boundary c will have limited smoothness, even though the coefficients in (3.2) may be C^∞ . The free boundary aspect of the problem was studied for a 1-dimensional flow situation in [6] and further, for the special case of travelling wave solutions, in [7, 9].

To prove uniqueness and stability for weak solutions only the monotonicity of the isotherms ϕ_i is required. There are three essential steps needed which we outline briefly below. In a later section about the convergence estimates they will reappear in discrete form.

Let $\zeta = c_1 - c_2$ and $\beta_i = s_{1i} - s_{2i}$, $i \in \{1, \dots, m\}$, where (c_1, s_{1i}) and (c_2, s_{2i}) are two weak solutions of Problem CTM. First, set

$$\eta(x, t) = \begin{cases} 0, & t \in (\tau, T], \\ \zeta(x, t), & t \in (0, \tau), \end{cases} \quad (4.1)$$

where $\tau \in (0, T)$. Note that η is not in $W_2^{1,1}(Q_T)$, because of the lack of smoothness of c_1 and c_2 in time, and because of the discontinuity at $t = \tau$. Thus, it is not a valid test function for (3.14). This difficulty can be circumvented, however, by introducing Steklov means as described in [12]. Using the Steklov mean of η in (3.14) leads to an expression that contains the term

$$\int_{Q_\tau} \rho \sum_{i=1}^m \lambda_i \frac{\partial \beta_i}{\partial t} \zeta. \quad (4.2)$$

Next, multiplying (3.10) by η defined by (4.1) gives

$$\frac{\partial \beta_i}{\partial t} \zeta = k\{\phi_i(c_1) - \phi_i(c_2)\}\zeta - k\beta_i\zeta \geq -k\beta_i\zeta, \quad (4.3)$$

where we have used the monotonicity of the isotherms. Then (4.2) can be estimated

from below by

$$-k \int_{Q_T} \rho \sum_{i=0}^m \lambda_i \beta_i \zeta. \quad (4.4)$$

Thirdly, in (3.14), we set

$$\eta(x, t) = \begin{cases} 0, & t \in (\tau, T], \\ -\int_t^\tau \zeta(x, s) ds, & t \in (0, \tau). \end{cases} \quad (4.5)$$

This gives an expression which contains a term similar to (4.4). After some technicalities and a Gronwall argument we obtain [6, 11]:

Theorem 4.1 *Let hypothesis (H1) be satisfied. Then Problem CTM has a unique weak solution.*

At the expense of some additional conditions it is possible to extend the uniqueness proof and to obtain a Lipschitz stability result for the difference in the $V_2^{1,0}(Q_T)$ norm.

Assume

$$(H2a) \quad \bar{q} \text{ and } \frac{\partial \theta}{\partial t} \text{ are independent of time;}$$

$$(H2b) \quad \frac{\partial}{\partial t}(\theta D) \text{ is positive definite a.e. in } Q_T \text{ and } \frac{\partial}{\partial t} \theta \leq 0 \text{ in } \Omega.$$

Then we obtain [6, 11]:

Theorem 4.2 *Let (c_1, s_{1i}) and (c_2, s_{2i}) , $i \in \{1, \dots, m\}$ denote the weak solution of Problem CTM corresponding to the data $\{c_{01}, s_{01i}, F_1\}$ and $\{c_{02}, s_{02i}, F_2\}$, respectively, and assume (H2) hold. Then there exists a constant $C > 0$ such that*

$$|c_1 - c_2|_{Q_T} \leq C \left\{ \|c_{01} - c_{02}\| + \sum_{i=1}^m \|\rho(s_{01i} - s_{02i})\| + \|F_1 - F_2\|_{L^\infty(S_{1T})} \right\}. \quad (4.6)$$

Remark. Using expression (3.3) for the hydrodynamic dispersion matrix, hypotheses (H2) are obviously fulfilled for the case of stationary water distribution (θ) and flow (\bar{q}).

Existence of weak, strong, and classical solutions was also established in [6] and [11]. Here we make some remarks in the direction of classical solutions. When the isotherms satisfy in addition to the monotonicity (H1a), the conditions (for $i \in \{1, \dots, m\}$)

$$\phi_i(0) = 0, \quad \phi_i(s) > 0 \quad \text{for } s > 0, \quad (4.7)$$

$$\phi_i \in C^p([0, \infty)) \cap C_{loc}^1((0, \infty)) \quad \text{for some } p \in (0, 1), \quad (4.8)$$

(such as the Freundlich isotherm (3.9)), and if the coefficients and initial/boundary data in Problem CTM are sufficiently smooth (e.g. $c_0 \in C^{2+p}(\bar{\Omega})$, $s_{0i} \in C^p(\bar{\Omega})$, $F = \alpha c_f$ with $c_f \geq 0$ and $c_f \in L^\infty(S_{1T})$, and other technical conditions), then

$$c \in C^{2+p, 1+p/2}(\bar{Q}_T) \quad \text{and} \quad s_i \in C^{p, p+1}(\bar{Q}_T). \quad (4.9)$$

Note that if one of the isotherms is of Freundlich type (3.9), then (4.9) is the optimal global regularity. Even if the coefficients in (3.2) (θ, ϕ, q and D) were C^∞ , this would only imply

$$c, s_i \in C^\infty(\{c > 0\} \cap Q_T).$$

For future reference, we note that (4.9) implies that c is continuously differentiable in time, and twice continuously differentiable in space, c_t and the second-order spatial derivatives of c are Hölder continuous in time with exponent $\frac{p}{2}$ and in space with exponent p , and the first-order spatial derivatives of c are Hölder continuous in time

with exponent $\frac{1+p}{2}$.

5 The CGFEM for Non-Equilibrium Adsorption

In this section we discuss the numerical approximation of solutions to (3.2), (3.10) by the CGFEM. For simplicity, assume $m = 1$ and $s_1 \equiv s$, so that $\lambda_1 = 1$ and $A \equiv s$.

We will make the following assumptions:

(H3a) The data and coefficients are sufficiently smooth so that (4.9) holds.

(H3b) The isotherm ϕ satisfies (H1a), (4.7), and (4.8).

(H3c) $\mathcal{S} = S_2$, with $D\nabla c \cdot n = 0$ on \mathcal{S} .

(H3d) θ and \bar{q} are independent of time.

(H3e) $D = D(\bar{q})$ is symmetric and positive definite.

For convenience, we will assume Problem CTM is Ω -periodic; i.e., we assume all functions involved are spatially Ω -periodic. This assumption is reasonable since the no-flow boundary conditions (H3c) are generally treated by reflection, and we are primarily interested in interior flow patterns and not boundary effects.

Let $0 = t^0 < t^1 < \dots < t^M = T$ be a given sequence, with $\Delta t^n = t^n - t^{n-1}$. Define $f^n(\cdot) = f(\cdot, t^n)$. Let $h > 0$ and M_h be a finite dimensional subspace of $W_2^1(\Omega)$ consisting of continuous, piecewise polynomials of degree at most one on a quasi-uniform mesh of diameter less than or equal to h .

In the CGFEM, we approximate $c(x, t^n)$ and $s(x, t^n)$ by functions C^n and S^n in M_h . Writing (3.2) in nondivergence form and applying (3.1), we obtain

$$\theta c_t + \rho s_t + \bar{q} \cdot \nabla c - \nabla \cdot (\theta D \nabla c) = 0 . \quad (5.1)$$

Let τ denote the unit vector in the direction (\bar{q}, θ) and set

$$\psi = (|\bar{q}|^2 + |\theta|^2)^{\frac{1}{2}} . \quad (5.2)$$

Then

$$\psi c_\tau \equiv \theta c_t + \bar{q} \cdot \nabla c \quad (5.3)$$

and (5.1) can be written as

$$\psi c_\tau - \nabla \cdot (\theta D \nabla c) + \rho s_t = 0 . \quad (5.4)$$

Let

$$\hat{x} = x - \frac{\bar{q}(x)}{\theta(x)} \Delta t , \quad (5.5)$$

and let $\hat{f}(x) \equiv f(\hat{x})$ for a given function f . Approximate ψc_τ by the backward difference

$$\psi c_\tau(x, t^n) \approx \theta(x) \frac{c(x, t^n) - c(\hat{x}, t^{n-1})}{\Delta t} . \quad (5.6)$$

Let

$$\sigma^n(x) = \psi(x) c_\tau^n(x) - \theta(x) \frac{c^n(x) - c(\hat{x}, t^{n-1})}{\Delta t} , \quad (5.7)$$

and

$$\omega^n(x) = s_t^n(x) - \frac{s^n(x) - s^{n-1}(x)}{\Delta t} . \quad (5.8)$$

Then (5.4) can be written

$$\theta \frac{c^n - \hat{c}^{n-1}}{\Delta t} - \nabla \cdot (\theta D \nabla c^n) + \rho \frac{s^n - s^{n-1}}{\Delta t} + \sigma^n + \rho \omega^n = 0, \quad (5.9)$$

and (3.10) can be written

$$\rho \frac{s^n - s^{n-1}}{\Delta t} = k \rho (\phi(c^n) - s^n) - \rho \omega^n. \quad (5.10)$$

Initially, set $C^0 = \tilde{C}^0 \in M_h$, where $\tilde{C}(x, t)$ is the θ -weighted L^2 -projection defined by

$$(\theta \tilde{C}(\cdot, t), \chi) = (\theta c(\cdot, t), \chi), \quad \chi \in M_h. \quad (5.11)$$

Furthermore, set $S^0 = \tilde{S}^0 \in M_h$, where $\tilde{S}(x, t)$ is the ρ -weighted L^2 -projection

$$(\rho \tilde{S}(\cdot, t), \chi) = (\rho s(\cdot, t), \chi), \quad \chi \in M_h. \quad (5.12)$$

For $n = 1, 2, \dots, M$, define $C^n \in M_h$, $S^n \in M_h$ by

$$\begin{aligned} & \left(\theta \frac{C^n - \hat{C}^{n-1}}{\Delta t}, \chi \right) + \left(\rho \frac{S^n - S^{n-1}}{\Delta t}, \chi \right) \\ & + (\theta D \nabla C^n, \nabla \chi) = 0, \quad \chi \in M_h, \end{aligned} \quad (5.13)$$

and

$$\left(\rho \frac{S^n - S^{n-1}}{\Delta t}, v \right) = k(\rho(\phi(C^n) - S^n), v), \quad v \in M_h. \quad (5.14)$$

Equations (5.13) and (5.14) are obtained by multiplying (5.9) and (5.10) by test functions χ and v in M_h , respectively, integrating (5.9) by parts, and substituting C^n for c^n , and S^n for s^n .

Existence and uniqueness of C^n and S^n follows from standard results found in [13]. Let I denote the dimension of M_h , and let $\{\psi_j(x)\}_{j=1}^I$ denote the standard nodal

basis. Note that (5.13) and (5.14) is equivalent to finding vectors $\mathcal{C}^n = \{C_j^n\}_{j=1}^I$ and $\mathcal{S}^n = \{S_j^n\}_{j=1}^I$, where $C^n(x) = \sum_{j=1}^I C_j^n \psi_j(x)$, $S^n = \sum_{j=1}^I S_j^n \psi_j(x)$, with \mathcal{C}^0 and \mathcal{S}^0 determined by (5.11) and (5.12), and for $n \geq 1$,

$$\begin{aligned} (A_1 + \Delta t B) \mathcal{C}^n + (1 + k\Delta t)^{-1} k\Delta t \Phi(\mathcal{C}^n) \\ = \hat{A}_1 \mathcal{C}^{n-1} + (1 + k\Delta t)^{-1} k\Delta t A_2 \mathcal{S}^{n-1}, \end{aligned} \quad (5.15)$$

$$(1 + k\Delta t) A_2 \mathcal{S}^n = A_2 \mathcal{S}^{n-1} + k\Delta t \Phi(\mathcal{C}^n). \quad (5.16)$$

Here $\Phi(\mathcal{C}^n) = \{(\rho\phi(C^n), \psi_j)\}_{j=1}^I$, A_1 , \hat{A}_1 , and A_2 are mass matrices with entries $(\theta\chi_i, \chi_j)$, $(\theta\hat{\chi}_i, \chi_j)$, and $(\rho\chi_i, \chi_j)$, respectively, and B is the stiffness matrix with entries $(\theta D\nabla\chi_i, \nabla\chi_j)$. Note that (5.15) can be written in the form $F(\mathcal{C}^n) = 0$. Since $A_1 + \Delta t B$ is positive definite and the components of $\Phi(\mathcal{C}^n)$ are continuous and monotone increasing, F is continuous and monotone increasing, and the existence and uniqueness of \mathcal{C}^n follows. The existence and uniqueness of \mathcal{S}^n then follows from (5.16) since A_2 is also positive definite.

6 Error Estimates

In this section we analyze the method given by (5.11)-(5.14). In the arguments that follow, K will denote a generic positive constant and ϵ a small positive constant, independent of h and Δt . We will also employ the well-known inequality

$$ab \leq \frac{1}{2\epsilon} a^2 + \frac{\epsilon}{2} b^2, \quad a, b, \epsilon \in \mathbb{R}, \quad \epsilon > 0.$$

A standard argument used in finite element analysis of parabolic equations is to compare the approximate solution to an elliptic projection [17]. This technique leads

to optimal rates of convergence in the norm $L^\infty(0, T; L^2(\Omega))$ as long as the solution is sufficiently smooth. In particular, when approximating by piecewise polynomials of degree one, one must have that c_t lies in the space $L^2(0, T; W_2^2(\Omega))$ to obtain h^2 accuracy in space. In the problem considered here, we are not guaranteed this much smoothness on the solution; in particular, we will only assume the smoothness given by (4.9). Thus, we will compare our approximate solutions to the L^2 -projections given by (5.11) and (5.12). This will reduce the provable rate of convergence from h^2 to h .

Let $\zeta = C - \tilde{C}$, $\xi = c - \tilde{C}$, where \tilde{C} is given by (5.11), and let $\beta = S - \tilde{S}$, where \tilde{S} is given by (5.12). Subtract (5.9) from (5.13), and (5.10) from (5.14), and use (5.11) and (5.12) to obtain

$$\begin{aligned} & \left(\theta \frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \chi \right) + (\theta D \nabla \zeta^n, \nabla \chi) + \left(\rho \frac{\beta^n - \beta^{n-1}}{\Delta t}, \chi \right) \\ &= (\sigma^n, \chi) + \left(\theta \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \chi \right) + (\theta D \nabla \xi^n, \nabla \chi) \\ & \quad + \left(\theta \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \chi \right) + (\rho \omega^n, \chi), \quad \chi \in M_h, \end{aligned} \quad (6.1)$$

and

$$\left(\rho \frac{\beta^n - \beta^{n-1}}{\Delta t}, v \right) = k(\rho(\phi(C^n) - \phi(c^n) - \beta^n), v) + (\rho \omega^n, v), \quad v \in M_h, \quad (6.2)$$

where σ^n is given by (5.7) and ω^n by (5.8).

We will derive an error estimate by taking $\chi = \zeta^n$ in (6.1), multiplying by Δt , and summing on n . We must first obtain a lower bound for the β term in (6.1) in terms of ζ , ξ , ω , and σ . To begin, following the uniqueness arguments given in [6], we set

$v = \zeta^n$ in (6.2) and note that by the monotonicity of ϕ :

$$\begin{aligned}
\left(\rho \frac{\beta^n - \beta^{n-1}}{\Delta t}, \zeta^n \right) &= k(\rho(\phi(C^n) - \phi(c^n)), \zeta^n) \\
&\quad - k(\rho\beta^n, \zeta^n) + (\rho\omega^n, \zeta^n) \\
&= k(\rho(\phi(C^n) - \phi(c^n)), C^n - c^n) \\
&\quad + k(\rho(\phi(C^n) - \phi(c^n)), \xi^n) \\
&\quad - k(\rho\beta^n, \zeta^n) + (\rho\omega^n, \zeta^n) \\
&\geq -k(\rho\beta^n, \zeta^n) + k(\rho(\phi(C^n) - \phi(c^n)), \xi^n) \\
&\quad + (\rho\omega^n, \zeta^n). \tag{6.3}
\end{aligned}$$

Thus,

$$\begin{aligned}
\sum_{n=1}^M \left(\rho \frac{\beta^n - \beta^{n-1}}{\Delta t}, \zeta^n \right) \Delta t &\geq \sum_{n=1}^M [-k(\rho\beta^n, \zeta^n) + k(\rho(\phi(C^n) - \phi(c^n)), \xi^n)] \Delta t \\
&\quad + \sum_{n=1}^M (\rho\omega^n, \zeta^n) \Delta t. \tag{6.4}
\end{aligned}$$

Next, we seek a lower bound for the β term on the right side of (6.4).

To this end, we consider (6.1) with a discrete time-integral test function in analogy with (4.5). Let $\chi = \sum_{\ell=n}^M \zeta^\ell \Delta t$ in (6.1), multiply the result by Δt , and sum on n , $n = 1, \dots, M$. First, we observe

$$\begin{aligned}
&\sum_{n=1}^M \left(\theta \frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Delta t \\
&= \sum_{n=1}^M \left(\theta \zeta^n, \left[\sum_{\ell=n}^M \zeta^\ell - \sum_{\ell=n+1}^M \zeta^\ell \right] \right) \Delta t \\
&= \sum_{n=1}^M (\theta \zeta^n, \zeta^n) \Delta t, \tag{6.5}
\end{aligned}$$

by summation by parts (where the sum from $n + 1$ to M is understood to be zero if $n = M$) and because $\zeta^0 = 0$. Similarly, since $\beta^0 = 0$,

$$\begin{aligned} & \sum_{n=1}^M \left(\rho \frac{\beta^n - \beta^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Delta t \\ &= \sum_{n=1}^M (\rho \beta^n, \zeta^n) \Delta t. \end{aligned} \tag{6.6}$$

Furthermore,

$$\begin{aligned} & (\nabla \zeta^n) \cdot \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \\ &= \frac{1}{2} \frac{\left\| \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \right\|^2 - \left\| \sum_{\ell=n+1}^M \nabla \zeta^\ell \Delta t \right\|^2}{\Delta t} \\ & \quad + \frac{1}{2} \nabla \zeta^n \cdot \nabla \zeta^n \Delta t; \end{aligned}$$

thus

$$\begin{aligned} & \sum_{n=1}^M \left(\theta D \nabla \zeta^n, \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \right) \Delta t \\ &= \frac{1}{2} \left(\theta D \sum_{n=1}^M \nabla \zeta^n \Delta t, \sum_{n=1}^M \nabla \zeta^n \Delta t \right) \\ & \quad + \frac{1}{2} \sum_{n=1}^M (\theta D \nabla \zeta^n, \nabla \zeta^n) \Delta t^2. \end{aligned} \tag{6.7}$$

Using (6.6), (6.1) with $\chi = \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t$, (6.5), and (6.7), we obtain

$$\begin{aligned} & -k \sum_{n=1}^M (\rho \beta^n, \zeta^n) \Delta t \\ &= -k \sum_{n=1}^M \left(\rho \frac{\beta^n - \beta^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Delta t \\ &= k \sum_{n=1}^M \left\{ \left(\theta \frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) + \left(\theta D \nabla \zeta^n, \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \right) \right\} \end{aligned}$$

$$\begin{aligned}
& + \left(\theta D \nabla \xi^n, - \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \right) \\
& + \left(\sigma^n + \theta \left(\frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t} \right) \right. \\
& \quad \left. + \theta \left(\frac{\hat{\xi}^{n-1} - \zeta^{n-1}}{\Delta t} \right) + \rho \omega^n, - \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Big\} \Delta t \\
= & k \sum_{n=1}^M \left\{ (\theta \zeta^n, \zeta^n) + \frac{1}{2} (\theta D \nabla \zeta^n, \nabla \zeta^n) \Delta t \right. \\
& + \left(\theta D \nabla \xi^n, - \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \right) \\
& + \left(\sigma^n + \theta \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t} \right. \\
& \quad \left. + \theta \frac{\hat{\xi}^{n-1} - \zeta^{n-1}}{\Delta t} + \rho \omega^n, - \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Big\} \Delta t \\
& + \frac{k}{2} \left(\theta D \sum_{n=1}^M \nabla \zeta^n \Delta t, \sum_{n=1}^M \nabla \zeta^n \Delta t \right). \tag{6.8}
\end{aligned}$$

By assumption (H1b), we can bound the last term in (6.8) from below, replacing θD by ν . Substituting (6.8) into (6.4), we obtain the desired lower bound for the β term of (6.1).

Setting $\chi = \zeta^n$ in (6.1), multiplying by Δt and summing on n , and using the bounds given by (6.4) and (6.8), we obtain

$$\begin{aligned}
& \sum_{n=1}^M \left\{ \left(\theta \frac{\xi^n - \zeta^{n-1}}{\Delta t}, \zeta^n \right) + (\theta D \nabla \zeta^n, \nabla \zeta^n) \right. \\
& \quad \left. + k \left[(\theta \zeta^n, \zeta^n) + \frac{1}{2} (\theta D \nabla \zeta^n, \nabla \zeta^n) \Delta t \right] \right\} \Delta t \\
& \quad + \frac{k\nu}{2} \left[\left(\sum_{n=1}^M \nabla \zeta^n \Delta t, \sum_{n=1}^M \nabla \zeta^n \Delta t \right) + \left(\sum_{n=1}^M \zeta^n \Delta t, \sum_{n=1}^M \zeta^n \Delta t \right) \right] \\
\leq & \sum_{n=1}^M \left\{ k(\rho(\phi(c^n)) - \phi(C^n), \xi^n) + (\sigma^n, \zeta^n) + \left(\theta \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \zeta^n \right) \right\} \Delta t
\end{aligned}$$

$$\begin{aligned}
& + (\theta D \nabla \xi^n, \nabla \zeta^n) + \left(\theta \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \zeta^n \right) \\
& + k \left[\left(\sigma^n, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) + \left(\theta \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \right. \\
& \quad + \left(\theta D \nabla \xi^n, \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \right) + \left(\theta \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \\
& \quad \left. + \left(\rho \omega^n, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \right] \Delta t \\
& + \frac{k\nu}{2} \left(\sum_{n=1}^M \zeta^n \Delta t, \sum_{n=1}^M \zeta^n \Delta t \right) \\
& \equiv T_1 + \cdots + T_{11}.
\end{aligned} \tag{6.9}$$

We now estimate the terms T_1 through T_{11} .

By the Hölder continuity of ϕ , and Hölder's inequality

$$\begin{aligned}
T_1 &= k \sum_{n=1}^M (\rho(\phi(c^n) - \phi(C^n)), \xi^n) \Delta t \\
&\leq k \|\rho\|_\infty \sum_{n=1}^M \|\phi(c^n) - \phi(C^n)\|_{L^q(\Omega)} \|\xi^n\|_{L^r(\Omega)} \Delta t \\
&\leq k \|\rho\|_\infty \sum_{n=1}^M \left(\int_\Omega |\zeta^n - \xi^n|^{qp} dx \right)^{\frac{1}{q}} \|\xi^n\|_{L^r(\Omega)} \Delta t,
\end{aligned}$$

where

$$\frac{1}{q} + \frac{1}{r} = 1.$$

Choose $q = \frac{2}{p}$, then $r = \frac{1}{1 - \frac{p}{2}} \leq 2$, and

$$\begin{aligned}
T_1 &\leq K h^2 \sum_{n=1}^M (\|\xi^n\|^2 + \|\zeta^n\|^2)^{\frac{2}{q}} \Delta t + K h^{-2} \sum_{n=1}^M \|\xi^n\|_{L^r(\Omega)}^2 \Delta t \\
&\leq K h^2 \sum_{n=1}^M [\|\xi^n\|^{2p} + \|\zeta^n\|^{2p}] \Delta t + K h^{-2} \sum_{n=1}^M \|\xi^n\|_{L^r(\Omega)}^2 \Delta t \\
&\leq K h^2 \sum_{n=1}^M [\|\zeta^n\|^{2p} + \|\xi^n\|^{2p}] \Delta t + K h^{-2} \sum_{n=1}^M \|\xi^n\|^2 \Delta t.
\end{aligned}$$

Consider

$$\begin{aligned}
T_2 &= \sum_{n=1}^M (\sigma^n, \zeta^n) \Delta t \\
&= \Delta t \sum_{n=1}^M \int_{\Omega} \left[\psi(x) c_{\tau}(x, t^n) - \theta(x) \frac{c^n(x) - \hat{c}^{n-1}(x)}{\Delta t} \right] \zeta^n(x) dx.
\end{aligned}$$

Note that

$$\begin{aligned}
&\psi(x) c_{\tau}(x, t^n) - \theta(x) \frac{c^n(x) - \hat{c}^{n-1}(x)}{\Delta t} \\
&= \psi(x) c_{\tau}(x, t^n) - \psi(x) \frac{1}{\Delta \bar{\tau}} \int_{(\hat{x}, t^{n-1})}^{(x, t^n)} c_{\bar{\tau}}(s, t) d\bar{\tau} \\
&= \psi(x) \frac{1}{\Delta \bar{\tau}} \int_{(\hat{x}, t^{n-1})}^{(x, t^n)} [c_{\tau}(x, t^n) - c_{\bar{\tau}}(s, t)] d\bar{\tau},
\end{aligned}$$

where $\Delta \bar{\tau} = \sqrt{|x - \hat{x}|^2 + \Delta t^2}$, and, for x fixed, $c_{\bar{\tau}}$ denotes the directional derivative of c in the direction of the constant vector $(\theta(x), \bar{q}(x))$. For (s, t) between (\hat{x}, t^{n-1}) and (x, t^n) , using the Hölder continuity of c_t and c_x in space and time (see (4.9)), we find

$$\begin{aligned}
|c_{\bar{\tau}}(s, t) - c_{\tau}(x, t^n)| &= |\theta(x)(c_t(s, t) - c_t(x, t^n)) + \bar{q}(x) \cdot (\nabla c(s, t) - \nabla c(x, t^n))| \\
&\leq K [|s - x|^p + |t - t^n|^{\frac{p}{2}}] \\
&\leq K \Delta t^{\frac{p}{2}}.
\end{aligned}$$

Thus,

$$\begin{aligned}
T_2 &\leq \Delta t \sum_{n=1}^M \int_{\Omega} \left| \psi(x) c_{\tau}(x, t^n) - \theta(x) \frac{c^n(x) - \hat{c}^{n-1}(x)}{\Delta t} \right| |\zeta^n(x)| dx \\
&\leq \Delta t \sum_{n=1}^M K \Delta t^{\frac{p}{2}} \|\zeta^n\| \\
&\leq K \Delta t^p + K \sum_{n=1}^M \|\zeta^n\|^2 \Delta t.
\end{aligned}$$

For a function $g(x) \in W_2^1(\Omega)$, we note that

$$\|g - \hat{g}\| \leq K \Delta t \|\nabla g\|,$$

and using the fact that $(\theta \xi^n, \chi) = 0$ for $\chi \in M_h$, we obtain

$$\begin{aligned} T_3 &= \sum_{n=1}^M \left(\theta \frac{\xi^n - \hat{\xi}^{n-1}}{\Delta t}, \zeta^n \right) \Delta t \\ &= \sum_{n=1}^M \left(\theta \frac{\xi^{n-1} - \hat{\xi}^{n-1}}{\Delta t}, \zeta^n \right) \Delta t \\ &\leq K \sum_{n=1}^M \|\nabla \xi^{n-1}\|^2 \Delta t + K \sum_{n=1}^M \|\zeta^n\|^2 \Delta t. \end{aligned}$$

Moreover,

$$\begin{aligned} T_4 &= \sum_{n=1}^M (\theta D \nabla \xi^n, \nabla \zeta^n) \Delta t \\ &\leq K \sum_{n=1}^M \|\nabla \xi^n\|^2 \Delta t + \epsilon \sum_{n=1}^M \|\nabla \zeta^n\|^2 \Delta t. \end{aligned}$$

Similar to the estimate for T_3 ,

$$\begin{aligned} T_5 &\leq \sum_{n=1}^M \left(\theta \frac{\hat{\xi}^{n-1} - \zeta^{n-1}}{\Delta t}, \zeta^n \right) \Delta t \\ &\leq K \sum_{n=1}^M \|\zeta^n\|^2 \Delta t + \epsilon \sum_{n=1}^M \|\nabla \zeta^{n-1}\|^2 \Delta t. \end{aligned}$$

Similar to the estimate for T_2 ,

$$\begin{aligned} T_6 &= k \sum_{n=1}^M \left(\sigma^n, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Delta t \\ &= k \sum_{n=1}^M \left(\sigma^n, \sum_{\ell=1}^M \zeta^\ell \Delta t - \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right) \Delta t \\ &\leq K \Delta t^p + \epsilon \left\| \sum_{\ell=1}^M \zeta^\ell \Delta t \right\|^2 \\ &\quad + K \sum_{n=1}^M \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|^2 \Delta t. \end{aligned}$$

Similar to the estimates for T_3 , T_4 , and T_6 ,

$$\begin{aligned}
T_7 &= \sum_{n=1}^M \left(\theta \frac{\xi^{n-1} - \hat{\xi}^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Delta t \\
&\leq K \sum_{n=1}^M \|\nabla \xi^{n-1}\|^2 \Delta t + \epsilon \left\| \sum_{\ell=1}^M \zeta^\ell \Delta t \right\|^2 \\
&\quad + K \sum_{n=1}^M \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|^2 \Delta t,
\end{aligned}$$

and

$$\begin{aligned}
T_8 &= \sum_{n=1}^M \left(\theta D \nabla \xi^n, \sum_{\ell=n}^M \nabla \zeta^\ell \Delta t \right) \Delta t \\
&\leq K \sum_{n=1}^M \|\nabla \xi^n\|^2 \Delta t + \epsilon \left\| \sum_{\ell=1}^M \zeta^\ell \Delta t \right\|_1^2 \\
&\quad + K \sum_{n=1}^M \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|_1^2 \Delta t.
\end{aligned}$$

Before estimating T_9 , we note that, for a spatially periodic, L^2 function g , it is shown in [4] that

$$\begin{aligned}
\left\| \frac{\hat{g} - g}{\Delta t} \right\|_{-1} &\equiv \sup_{f \in W_2^1(\Omega), f \neq 0} \left[\frac{1}{\|f\|_1} \int_{\Omega} \frac{\hat{g}(x) - g(x)}{\Delta t} f(x) dx \right] \\
&\leq K \|g\|.
\end{aligned} \tag{6.10}$$

Thus,

$$\begin{aligned}
T_9 &= \sum_{n=1}^M \left(\theta \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t}, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Delta t \\
&\leq K \sum_{n=1}^M \left\| \frac{\hat{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t} \right\|_{-1} \left\| \sum_{\ell=n}^M \zeta^\ell \Delta t \right\|_1 \Delta t \\
&\leq K \sum_{n=1}^M \|\zeta^{n-1}\|^2 \Delta t + \epsilon \left\| \sum_{\ell=1}^M \zeta^\ell \Delta t \right\|_1^2 \\
&\quad + K \sum_{n=1}^M \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|_1^2 \Delta t.
\end{aligned}$$

For the estimate of T_{10} , consider

$$\begin{aligned}\omega^n &= s_t(\cdot, t^n) - \frac{s^n - s^{n-1}}{\Delta t} \\ &= \frac{1}{\Delta t} \int_{t^{n-1}}^{t^n} [s_t(\cdot, t^n) - s_t(\cdot, t)] dt.\end{aligned}$$

By the Hölder continuity of s_t , we obtain

$$\begin{aligned}\frac{1}{\Delta t} \int_{t^{n-1}}^{t^n} [s_t(\cdot, t^n) - s_t(\cdot, t)] dt \\ \leq \frac{K}{\Delta t} \int_{t^{n-1}}^{t^n} |t - t^n|^p dt \\ \leq K \Delta t^p.\end{aligned}$$

Thus,

$$\begin{aligned}T_{10} &= \sum_{n=1}^M \left(\rho \omega^n, \sum_{\ell=n}^M \zeta^\ell \Delta t \right) \Delta t \\ &\leq K \Delta t^{2p} + \epsilon \left\| \sum_{\ell=1}^M \zeta^\ell \Delta t \right\|^2 + K \sum_{n=1}^M \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|^2 \Delta t.\end{aligned}$$

Finally,

$$\begin{aligned}T_{11} &= \frac{k\nu}{2} \left(\sum_{n=1}^M \zeta^n \Delta t, \sum_{n=1}^M \zeta^n \Delta t \right) \\ &\leq K \sum_{n=1}^M \|\zeta^n\|^2 \Delta t + \epsilon \left\| \sum_{n=1}^M \zeta^n \Delta t \right\|^2.\end{aligned}$$

Combining the estimates for T_1 – T_{11} with (6.9), and using the fact that

$$\sum_{n=1}^M \left(\theta \frac{\zeta^n - \zeta^{n-1}}{\Delta t}, \zeta^n \right) \Delta t \geq \frac{1}{2} (\theta \zeta^M, \zeta^M)$$

and the estimate

$$\|\xi(\cdot, t)\| + h \|\xi(\cdot, t)\|_1 \leq K h^2 \|c(\cdot, t)\|_2$$

(here we use the quasi-uniformity assumption on the mesh), we find

$$\begin{aligned}
& \frac{1}{2}(\theta\zeta^M, \zeta^M) \\
& + \sum_{n=1}^M \left[(D\nabla\zeta^n, \nabla\zeta^n) + k(\theta\zeta^n, \zeta^n) + \frac{1}{2}(D\nabla\zeta^n, \nabla\zeta^n)\Delta t \right] \Delta t \\
& + \frac{k\nu}{2} \left[\left(\sum_{n=1}^M \nabla\zeta^n \Delta t, \sum_{n=1}^M \nabla\zeta^n \Delta t \right) + \left(\sum_{n=1}^M \zeta^n \Delta t, \sum_{n=1}^M \zeta^n \Delta t \right) \right] \\
& \leq Kh^2 \sum_{n=1}^M \|\zeta^n\|^{2p} \Delta t + K \sum_{n=1}^M \|\zeta^n\|^2 \Delta t + K \Delta t^{2p} + K \Delta t^p + Kh^2 \\
& + \epsilon \sum_{n=1}^M \|\zeta^n\|_1^2 \Delta t + K \sum_{n=1}^M \left\| \sum_{\ell=1}^{n-1} \zeta^\ell \Delta t \right\|_1^2 \Delta t \\
& + \epsilon \left\| \sum_{n=1}^M \zeta^n \Delta t \right\|_1^2. \tag{6.11}
\end{aligned}$$

We now hide terms multiplied by ϵ , and define

$$g^n = (\zeta^n, \zeta^n) + \left\| \sum_{\ell=1}^n \zeta^\ell \Delta t \right\|_1^2.$$

The L^2 stability of C^n can be demonstrated using essentially the same arguments given above; i.e., we set χ and $v = C^n$ in (5.13) and (5.14), and use the monotonicity of ϕ . We then set $\chi = \sum_{\ell=n}^M C^\ell \Delta t$ in (5.13), multiply the result by Δt and sum on n , and sum by parts. The result is that $\|C^n\| \leq K\|C^0\|$ for each n , where K is independent of h and Δt . Thus, by the L^2 stability of \tilde{C} , we have

$$\|\zeta^n\|^{2p} \leq K.$$

Then, (6.11) implies

$$g^M \leq K(h^2 + \Delta t^p) + K \sum_{n=1}^M |g^n| \Delta t.$$

Applying Gronwall's Lemma and the triangle inequality, we obtain the following result:

Theorem 6.1 *Assume (H1a)-(H1f), (4.7)-(4.9), and (H3a)-(H3e) hold, then*

$$\max_n \|c^n - C^n\| \leq K(\Delta t^{\frac{p}{2}} + h).$$

Remark. When θ and \bar{q} are time-dependent (hence D is time-dependent), this introduces additional terms into the summation by parts arguments which lead to (6.5) and (6.7). In particular, we obtain terms involving discrete time differences on θ and θD . In this case, to derive error estimates we must assume these discrete differences satisfy assumptions analogous to those given in (H2b). To our knowledge, these assumptions do not have any physical justification.

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