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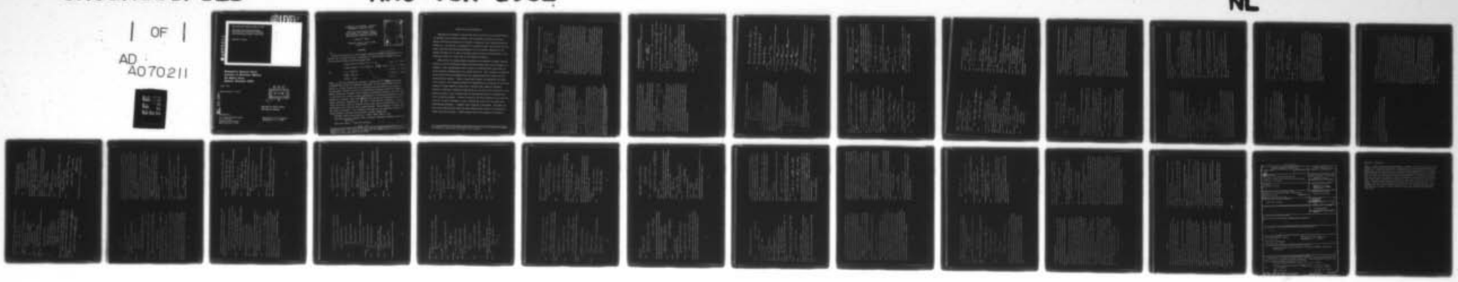

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EFFICIENT TIME-STEPPING METHODS FOR MISCIBLE DISPLACEMENT PROBLEMS WITH NONLINEAR BOUNDARY CONDITIONS

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ABSTRACT

Efficient procedures for time-stepping Galerkin methods for approximating the solution of a coupled nonlinear system ~~for $c = c(x,t)$ and $p = p(x,t)$~~ with nonlinear Neumann boundary conditions of the form

$$
(*)\qquad
\begin{aligned}
&\nabla\cdot[a(x,c)\{\nabla p-\gamma(x,c)\nabla c\}] \equiv -\nabla\cdot u = f_1, && x\in\Omega,\ t\in(0,T],\\
&\nabla\cdot[b(x,c,\nabla p)\nabla c] - u(x,c,\nabla p)\cdot\nabla c = \phi(x)\frac{\partial c}{\partial t} + f_2(c), && x\in\Omega,\ t\in(0,T],\\
&u\cdot\nu = g_1(x,t) && x\in\partial\Omega,\ t\in(0,T],\\
&b\frac{\partial c}{\partial \nu} = g(x,t,c) && x\in\partial\Omega,\ t\in(0,T],\\
&c(x,0) = c_0(x) && x\in\Omega,
\end{aligned}
$$

where $\Omega \subset \mathbb{R}^2$, are presented and analyzed. Systems like (*) are possible model systems for describing the miscible displacement of one incompressible fluid by another in a porous medium when flow conditions are prescribed on the boundary. The procedures involve the use of a preconditioned iterative method for approximately solving the different linear systems of equations arising at each time step in a discrete-time Galerkin method. Improvements in starting procedures over many methods are obtained. Some negative-index norm results are obtained which allow weaker smoothness assumptions on $\frac{\partial c}{\partial t}$ than in some previous treatments. Optimal order convergence rates are obtained in most cases for the methods which are computationally more efficient than standard methods. Work estimates of almost optimal order are obtained. The techniques developed are also applied to single nonlinear parabolic equations with nonlinear boundary conditions.

AMS(MOS) Subject Classifications: 65M15, 65N15, 65N30, 76.35

Key Words: Galerkin methods, Error estimates, Nonlinear boundary conditions, Fluid flow.

Work Unit Number 7 - Numerical Analysis.

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Significance and Explanation

Many physical problems in which fluid flow or heat flow is prescribed across the boundary of the region of interest can be modeled by nonlinear parabolic partial differential equations (or systems of equations) with nonlinear boundary conditions. An analysis is presented for a particular model system which has been used to describe the miscible displacement of oil by certain chemicals in the chemical flooding of oil wells to produce greater recovery from reservoirs. The techniques extend to a wide class of such physical problems.

Some results for single parabolic equations are extended to certain coupled systems of partial differential equations where optimal order error estimates are obtained. Next, approximation theory results are obtained which allow some reduced smoothness assumptions on the unknown functions. Also, analysis is presented which allows starting procedures which are computationally more efficient than in many earlier results. Finally, significant amounts of computation are saved by an iterative time-stepping procedure for approximating the solution of the large systems of linear equations produced by a Galerkin-type numerical procedure. Instead of factoring a different large matrix at each time step to solve the linear equations exactly, only one matrix must be factored and used as a preconditioner in an iterative procedure. Very few iterations are then required at each time step since the iterative procedure is just a stabilizing process for the underlying time-stepping procedure. A complete error analysis is presented. The paper contains work estimates which show the large computational savings of the preconditioned iterative technique. Almost optimal order work estimates are obtained.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

EFFICIENT TIME-STEPPING METHODS FOR MISCIBLE DISPLACEMENT PROBLEMS WITH NONLINEAR BOUNDARY CONDITIONS

Richard E. Ewing

1. Introduction.

We shall consider efficient procedures for time-stepping Galerkin methods for approximating the solution of a problem arising in the miscible displacement of one incompressible fluid by another in a porous medium. A set of equations which has been used to model the concentration $c = c(x,t)$ of the fluids and the pressure $p = p(x,t)$ [18, 19, 12] is given by

$$\text{(1.1)}\quad \begin{aligned} &a)\quad \nabla\cdot[a(\nabla p-\gamma\nabla d)] \equiv -\nabla\cdot u = f_1 , && x\in\Omega,\ t\in(0,T],\\ &b)\quad \nabla\cdot[b\nabla c-uc] = \phi\frac{\partial c}{\partial t} + f_1\hat{c} , && x\in\Omega,\ t\in(0,T], \end{aligned}$$

where $x\in\Omega\subset\mathbb{R}^2$ (the reservoir Ω is a bounded domain with boundary $\partial\Omega$) and where $a = a(x,c)$, $\gamma=\gamma(x,c)$, $d=d(x)$, $f_1=f_1(x,t)$, $\hat{c}$, $\phi=\phi(x)$, and $b=b(x,c,\nabla p)$ (or $b=b(x,c)$ or $b=b(x)$ in other cases) are prescribed. See [18, 19, 12] for the physical significance of the functions. We assume that (1.1) holds subject to boundary conditions consisting of the specification of the Darcy velocity at the boundary, the total flow across the boundary, and an initial concentration. We thus assume boundary conditions for (1.1) of the form

$$\text{(1.2)}\quad \begin{aligned} &a)\quad u\cdot\nu = g_1(x,t) , && x\in\partial\Omega,\ t\in(0,T],\\ &b)\quad b\frac{\partial c}{\partial\nu} - u\cdot\nu = g_2(x,t), && x\in\partial\Omega,\ t\in(0,T] ,\\ &c)\quad c(x,0) = c_0(x) , && x\in\Omega . \end{aligned}$$

We are interested in Galerkin or finite element approximations of the solution of (1.1)-(1.2). We shall look for functions in finite dimensional subspaces of $H^1(\Omega)$ which satisfy the weak formulation of (1.1)-(1.2). We note that if $c(x,t) \equiv 1$, then (1.1.a) and (1.1.b) are identical. This would indicate a strong relationship between the subspaces used for (1.1.a) and (1.1.b). Since the pressure changes rapidly near input or outlet wells and the concentration changes rapidly along a moving front, we would like to use very different subspaces for the two equations (and two different unknowns). Thus instead of using the divergence form (1.1), we shall consider the non-divergence form with associated boundary conditions given by

$$\text{(1.3)}\quad \begin{aligned} &a)\quad \nabla\cdot[a(\nabla p-\gamma\nabla d)] \equiv -\nabla\cdot u = f_1 , && x\in\Omega,\ t\in(0,T] ,\\ &b)\quad \nabla\cdot[b\nabla c] - u\cdot\nabla c = \phi\frac{\partial c}{\partial t} + f_1(\hat{c}-c), && x\in\Omega,\ t\in(0,T] ,\\ &c)\quad u\cdot\nu = g_1(x,t) , && x\in\partial\Omega,\ t\in(0,T] ,\\ &d)\quad b\frac{\partial c}{\partial\nu} = g(x,t,c) , && x\in\partial\Omega,\ t\in(0,T] ,\\ &e)\quad c(x,0) = c_0(x) , && x\in\Omega , \end{aligned}$$

where

$$\text{(1.4)}\quad g(x,t,c) = u\cdot\nu c + g_2(x,t) = g_1(x,t)c + g_2(x,t)$$

from (1.2) (a) and (b) above. Thus, by considering the non-divergence form of the equation, we are naturally led to the use of boundary conditions which depend upon c . Under the assumption that f_1 corresponds to smoothly distributed sources and sinks, the analysis of the f_1 terms follows immediately from the other analysis. Thus, for simplicity of presentation, we shall assume $f_1 \equiv 0$ in what follows.

We are interested in efficient procedures for time-stepping Galerkin methods which approximate the solution of (1.3). Our modification of the usual Galerkin method consists of using an iterative method employing a fixed preconditioning matrix to approximately solve the linear (lagging or extrapolating values in coefficients produces linear rather than nonlinear) algebraic equations at each time step. We preserve the accuracy inherent in the underlying Galerkin method, and we obtain very nearly optimal possible work estimates.

The analysis of nonlinear boundary conditions involves several techniques which differ from the analysis of homogeneous boundary conditions considered in [11,12]. Although the literature contains some treatments of parabolic equations with nonlinear boundary conditions [5, 16], there is little analysis for coupled partial differential equations of the form (1.3). The goals of this paper are to extend the analysis of nonlinear boundary conditions of [5, 16] to the systems

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described above to obtain optimal order L^2 error estimates, to weaken some of the smoothness and starting condition assumptions of [6, 11, 16], and to present and analyze efficient numerical procedures for both coupled systems and single parabolic equations with nonlinear boundary conditions.

Since the techniques which we develop for the coupled system (1.3) will also treat single nonlinear parabolic problems with nonlinear boundary conditions, we shall present some results for single equations also. We shall consider the problem of determining $c = c(x,t)$ satisfying

$$\text{(1.5)}\quad \begin{aligned} &a) \quad \nabla\cdot[b(x,c)\nabla c] - u(x,c)\cdot\nabla c = \phi(x)\frac{\partial c}{\partial t} + f_1(x,c), \quad x \in \Omega,\ t \in (0,T], \\ &b) \quad b(x,c)\frac{\partial c}{\partial \nu} = g(x,t,c), \quad x \in \partial\Omega,\ t \in (0,T], \\ &c) \quad c(x,0) = c_0(x), \quad x \in \Omega. \end{aligned}$$

Again, for simplicity, we shall assume $f_1 \equiv 0$ in (1.5).

In Section 2 we introduce two families of finite element spaces which we use to approximate our unknown functions and present the smoothness assumptions for the functions and domain of our problem. We also define elliptic projections for c and p, derive approximation theory results for these projections, and present the basic Galerkin approximations for (1.3). In Section 3 we present our iterative modifications of the basic methods and analyze the effect of the iterative approximation on a single time step. In Section 4 we obtain global error estimates for the various methods described in Sections 2 and 3. Section 5 contains a brief discussion of the estimates of the computational complexity of the methods presented in this paper.

2. Preliminaries and Description of Galerkin Methods

Let $(\phi,\psi) = \int_\Omega \phi\psi\, dx$ and $\|\phi\|^2 = (\phi,\phi)$. Let $W_s^k(\Omega)$ be the Sobolev space on Ω with norm

$$\|\phi\|_{W_s^k} \left(\sum_{|\alpha|\le k} \left\| \frac{\partial^\alpha \phi}{\partial x^\alpha} \right\|^s_{L^s(\Omega)} \right)^{1/s},$$

with the usual modification for $s = \infty$. When $s = 2$, let $\|\phi\|_{W_2^k} = \|\phi\|_{H^k} = \|\phi\|_k$.

If $\mathbf{F} = (F_1, F_2)$, write $\|\mathbf{F}\|_{W_s^k}$ in place of $\left(\|F_1\|^s_{W_s^k} + \|F_2\|^s_{W_s^k}\right)^{1/s}$. Let $H^s(\partial\Omega)$ denote the corresponding Sobolev space on $\partial\Omega$ with norm $\|\phi\|_{H^s(\partial\Omega)} \equiv |\phi|_s$ (with $|\phi| \equiv |\phi|_0$).

Let $\{M_h\}$ be a family of finite-dimensional subspaces of $H^1(\Omega)$ with the following property:

For $p = 2$ or $p = \infty$, there exist an integer $r \ge 2$ and a constant K_0 such that, for $1 \le q \le r$ and $\phi \in W_p^q(\Omega)$,

$$\text{(2.1)}\quad \inf_{\chi \in M_h} \{\|\phi-\chi\|_{W_p^0} + h\|\phi-\chi\|_{W_p^1}\} \le K_0\|\phi\|_{W_p^q} h^q .$$

Similarly, we define a family of finite-dimensional subspaces of $H^1(\Omega)$ called $\{N_h\}$ which satisfies the same property as $\{M_h\}$ with r replaced by s. We also assume that the families $\{M_h\}$ and $\{N_h\}$ satisfy the following so-called "inverse hypotheses": if $\phi \in M_h$ and $\psi \in N_h$,

$$\text{(2.2)}\quad \begin{aligned} &a) \quad \|\phi\|_{L^\infty(\Omega)} \le K_0 h^{-\frac{d}{2}}\|\phi\| = K_0 h^{-1}\|\phi\|, \\ &b) \quad \|\nabla\psi\|_{L^\infty(\Omega)} \le K_0 h^{-1}\|\nabla\psi\|, \\ &c) \quad \|\phi\|_1 \le K_0 h^{-1}\|\phi\| . \end{aligned}$$

Restrict Ω as follows (with (S) denoting the collection of restrictions):

(S): 1) Ω is H^2-regular; i.e., if

$$-\Delta v + \theta v = \zeta\ ,\quad x \in \Omega\ ,\quad \theta = 0 \text{ or } 1\ ,$$

$$\frac{\partial v}{\partial \nu} = \eta\ ,\quad x \in \partial\Omega,$$

and $(\zeta,1) + (\eta,1) = 0$, if $\theta = 0$,

then $\|v\|_2 \le K(\Omega)(\|\zeta\| + |\eta|_{1/2})$;

2) $\partial\Omega$ is Lipschitz.

For the physical problem, the coefficients are well-behaved if the approximation for c lies between two previously determined constants and if the approximation for ∇p remains bounded. Since we shall obtain $L^\infty(\Omega)$ estimates from our procedures, we shall, without loss of generality, assume that these constraints are met and will assume uniform bounds for the coefficients. For a careful treatment of similar problems where corresponding uniform assumptions are not made, see [11, 12].

Assume the following regularity for a, γ, b, ϕ, and u :

(Q): 1. There exist uniform constants such that

a) $0 < a_* \le a(x,q_1) \le a^* \le K_1$,

b) $0 < \phi_* \le \phi(x) \le \phi^* \le K_1$,

c) $0 < b_* \le b(x,q_1,q_2,q_3) \le K_1$,

(2.3) d) $|\gamma(x,q_1)| \le K_1$,

e) $|\nabla d| \le K_1$,

f) $|u_i(x,q_1,q_2)| \le K_1(1 + |q_2|)$, $i = 1,2$,

g) $|g(x,c)| \le K_1$,

for $q_1,q_2,q_3 \in \mathbb{R}$.

2. Let the derivatives of $a=a(x,c)$, $b=b(x,c,\nabla p)$, $\gamma=\gamma(x,c)$, $u_i=u_i(x,c,q)$, and $g=g(x,c)$ satisfy the following assumptions: for $i = 1,2$, $q_1,q_2 \in \mathbb{R}$, and $q_3 \in \mathbb{R}^2$,

$$\left|\frac{\partial a}{\partial x_i}(x,q_1)\right| + \left|\frac{\partial a}{\partial c}(x,q_1)\right| + \left|\frac{\partial^2 a}{\partial x_i \partial c}(x,q_1)\right| + \left|\frac{\partial^2 a}{\partial c^2}(x,q_1)\right|$$

$$+ \left|\frac{\partial \gamma}{\partial c}(x,q_1)\right| + \left|\frac{\partial b}{\partial c}(x,q_1,q_3)\right| + \left|\frac{\partial b}{\partial \nabla p}(x,q_1,q_3)\right| + \left|\frac{\partial^2 b}{\partial c^2}(x,q_1,q_2)\right|$$

(2.4)

$$+ \left|\frac{\partial u_i}{\partial c}(x,q_1)\right| + \left|\frac{\partial u_i}{\partial x_i}(x,q_1)\right| + \left|\frac{\partial g}{\partial t}(t,q_1)\right| + \left|\frac{\partial g}{\partial c}(t,q_1)\right|$$

$$+ \left|\frac{\partial^2 g}{\partial t \partial c}(t,q_1)\right| + \left|\frac{\partial^2 g}{\partial c^2}(t,q_1)\right| \le M\ .$$

Define

(2.5) $$\|\psi\|_{W_p^q((a,b);X)} \equiv \|\|\psi(\cdot,t)\|_X\|_{W_p^q(a,b)}\ ,\quad 1 \le p,q \le \infty\ .$$

Let (p,c), the solution of (1.3) satisfy the following regularity assumptions:

(R) a) $\|c\|_{L^\infty(J;H^r)} + \left\|\frac{\partial c}{\partial t}\right\|_{L^2(J;H^{r-1})} \le K_2$,

b) $\|p\|_{L^\infty(J;H^s)} + \left\|\frac{\partial p}{\partial t}\right\|_{L^2(J;H^{s-1})} \le K_2$,

(2.6) c) $\|c\|_{L^\infty(J;H^3)} + \left\|\frac{\partial c}{\partial t}\right\|_{L^\infty(J;H^{2+\epsilon})} + \left\|\frac{\partial c}{\partial t}\right\|_{L^2(J;W_\infty^2)} \le K_2$, for some $\epsilon > 0$,

d) $\|p\|_{L^\infty(J;H^3)} + \left\|\frac{\partial p}{\partial t}\right\|_{L^2(J;W_\infty^2)} \le K_2$,

e) $\left\|\frac{\partial^2 c}{\partial t^2}\right\|_{L^\infty(J;H^1)} + \left\|\frac{\partial^2 p}{\partial t^2}\right\|_{L^\infty(J;H^1)} \le K_2$,

where $J \equiv (0,T]$.

The analysis will proceed, following Wheeler [21], using a pair of auxiliary elliptic problems. Let $\tilde{p} \in M_h$ be the elliptic projection of p into M_h defined by

(2.7) $$(a(\cdot,c(\cdot,t))\nabla\tilde{p},\nabla v) = (a(\cdot,c(\cdot,t))\nabla p,\nabla v) = (a(c)\gamma(c)\nabla d,\nabla v) + (g_1,v)\ ,\quad v \in M_h\ ,$$

for each $t \in J$, where

$$\frac{1}{|\Omega|}\int_{\Omega}(\tilde{p}(x,t) - p(x,t))dx = 0\,, \quad \text{for each } t \in J\,, \tag{2.8}$$

and where (p,c) is the solution of (1.3). The restrictions (S) imply the following result [8,21].

<u>Lemma 2.1</u>. There exists $K_3 = K_3(\Omega, a_*, K_0, K_1, K_2)$ such that for $2 \le q \le s$ and $t \in J$,

$$\|p - \tilde{p}\| + h\{\|\nabla(p - \tilde{p})\| + \|\nabla\frac{\partial(p - \tilde{p})}{\partial t}\|\} \le K_3 h^q\{\|p\|_q + \|\frac{\partial p}{\partial t}\|_q\}\,. \tag{2.9}$$

Let $\lambda > 0$ be chosen sufficiently large that the bilinear form

$$B(\phi,\chi) = (b(c,\nabla p)\nabla\phi, \nabla\chi) + (u(c,\nabla p)\cdot\nabla\phi, \chi) + \lambda(\phi,\chi) - (g(t,\phi),\chi) \tag{2.10}$$

satisfies

$$B(\phi,\phi) \ge K_*\|\phi\|_1^2\,, \qquad \phi \in M_h\,. \tag{2.11}$$

Let $\tilde{c} \in M_h$ be the elliptic projection of c into M_h, defined by

$$B(\tilde{c},w) = B(c,w) = -(\phi\frac{\partial c}{\partial t}, w) + \lambda(c,w)\,, \qquad w \in M_h\,, \tag{2.12}$$

for each $t \in J$. Then, using the techniques of [5,8,16,21] (see also the proof of Lemma 2.4, below), we can obtain the following lemma.

<u>Lemma 2.2.</u> There exists $K_4 = K_4(\Omega, b_*, \lambda, K_0, K_1, K_2, K_*, M)$ such that for $2 \le q \le r$

a) $$\|\tilde{c}-c\|_{L^2(J;L^2)} + \left\|\frac{\partial(\tilde{c}-c)}{\partial t}\right\|_{L^2(J;L^2)} + h\|\tilde{c}-c\|_{L^2(J;H^1)}$$

$$\le K_4 h^q\{\|c\|_{L^2(J;H^q)} + \left\|\frac{\partial c}{\partial t}\right\|_{L^2(J;H^q)}\}\,, \tag{2.13}$$

b) $$\|\tilde{c} - c\|_{L^\infty(J;L^2)} \le K_4 h^q\|c\|_{L^\infty(J;H^q)}\,.$$

We also make the assumptions on $\{M_h\}$, $\{N_h\}$, c, and p that there exists a constant K_5 such that

$$\|\nabla\tilde{p}\|_{L^\infty(J;L^\infty)} + \left\|\frac{\partial\tilde{p}}{\partial t}\right\|_{L^\infty(J;H^1)} + \|c\|_{L^\infty(J;W^1_\infty)}$$
$$+ \left\|\frac{\partial\tilde{c}}{\partial t}\right\|_{L^\infty(J;H^1)} + \left\|\frac{\partial\tilde{c}}{\partial t}\right\|_{L^1(J;W^2_\infty)} \le K_5\,. \tag{2.14}$$

Sufficient conditions for (2.14) to hold can be found in [6, 21]. Also as in [4, 5, 6] we can obtain the following lemma.

<u>Lemma 2.3.</u> There exists a constant $K_6 = K_6(K_1, K_2, K_3, K_5)$ such that

$$\left\|\frac{\partial^2 c}{\partial t^2}\right\|_{L^\infty(J;H^1)} + \left\|\frac{\partial^2 \tilde{p}}{\partial t^2}\right\|_{L^\infty(J;H^1)} \le K_6\,. \tag{2.15}$$

In order to reduce to smoothness assumptions on c necessary to achieve our results when $r > 2$, we shall need to use some duality theory and obtain approximation theory results in negative-indexed norms. For these results, assume that Ω, a, b, γ, and q are sufficiently smooth [15] that for each $t \in J$, if

(2.16)

a) $$Lv \equiv -\nabla\cdot[b(c,\nabla p)\nabla v + u(c,\nabla p)v] + \lambda v = \phi_1\,, \quad x \in \Omega\,,$$

b) $$b(c,\nabla p)\frac{\partial v}{\partial\nu} + u(c,\nabla p)\cdot\nu\, v = \phi_2\,, \quad x \in \partial\Omega\,,$$

then

$$\|v\|_{k+2} \le K_7\{\|\phi_1\|_k + |\phi_2|_{k+\frac{1}{2}}\}\,. \tag{2.17}$$

If (2.16)-(2.17) holds, we shall say that Ω is H^{k+2}-regular. We note that by the trace theorem [15],

$$\left|\frac{\partial v}{\partial\nu}\right|_{k+\frac{1}{2}} + |v|_{k+\frac{3}{2}} \le K_8\|v\|_{k+2}\,. \tag{2.18}$$

Next define, for $k \ge 0$,

(2.19)

a) $\|\phi\|_{-k} \equiv \sup\{(\phi,\sigma) : \|\sigma\|_k = 1\}$,

b) $|\phi|_{-k} \equiv \sup\{(\phi,\sigma) : |\sigma|_k = 1\}$.

<u>Lemma 2.4.</u> If Ω is H^{k+2}-regular for $k \ge 1$, there exists a constant $K_9 = K_9(\Omega, b_*, \lambda, K_0, K_1, K_2, K_4, K_*, M)$ such that for $1 \le q \le r$ and $t \in J$,

$$\|c-\tilde{c}\|_{-k} + |c-\tilde{c}|_{-(k+\frac{1}{2})} + \left\|\frac{\partial(c-\tilde{c})}{\partial t}\right\|_{-k} \le K_9 h^{q+k}\{\|c\|_q + \left\|\frac{\partial c}{\partial t}\right\|_q\}\,. \tag{2.20}$$

Proof: Let $\xi = c - \tilde{c}$ and denote

(2.21) $$G(x,t) = \int_0^1 \frac{\partial g}{\partial c}(x,t,\theta c(x,t) + (1-\theta)\tilde{c}(x,t))d\theta.$$

Note that (2.12) can be written as

(2.22) $$B(\xi,\chi) = 0 , \quad \chi \in M_h .$$

Differentiating (2.22) with respect to t, we obtain

(2.23) $$B(\xi_t,\chi) = N(\chi) , \quad \chi \in M_h ,$$

where

(2.24)
$$N(\chi) \equiv -((\frac{\partial b}{\partial c}\frac{\partial c}{\partial t} + \frac{\partial b}{\partial \nabla p}\frac{\partial \nabla p}{\partial t}]\nabla\xi,\nabla\chi) - ([\frac{\partial u}{\partial c}\frac{\partial c}{\partial t} - \frac{\partial u}{\partial \nabla p}\frac{\partial \nabla p}{\partial t}]\cdot\nabla\xi,\chi)$$
$$+ (\{\frac{\partial g}{\partial t}(c) - \frac{\partial g}{\partial t}(\tilde{c})\} + \frac{\partial c}{\partial t}\{\frac{\partial g}{\partial c}(c) - \frac{\partial g}{\partial c}(\tilde{c})\},\chi)$$
$$\equiv -(\alpha_1\nabla\xi,\nabla\chi) - (\alpha_2\cdot\nabla\xi,\chi) + (\alpha_3,\chi) .$$

Let $\psi \in H^k(\Omega)$. Let $\varphi \in H^{k+2}(\Omega)$ be the solution of

(2.25)
a) $L\varphi \equiv -\nabla\cdot[b(c,\nabla p)\nabla\varphi + u(c,\nabla p)\varphi] + \lambda\varphi = \psi , \quad x \in \Omega ,$
b) $\hat{L}\varphi \equiv b(c,\nabla p)\frac{\partial\varphi}{\partial\nu} + u(c,\nabla p)\cdot\nu\varphi - G\varphi = 0 , \quad x \in \partial\Omega.$

Using smoothness assumptions from (Q) and (R), the H^{k+2}-regularity of Ω, and Lemma 2.2 from [5], we can obtain, as in [5],

(2.26) $$\|\varphi\|_{k+2} \le K_7 \|\psi\|_k .$$

Then from (2.25) we see that for $w \in M_h$,

(2.27)
$$(w,\psi) = -(w,\nabla\cdot[b(c,\nabla p)\nabla\varphi + u(c,\nabla p)\varphi]) + \lambda(w,\varphi)$$
$$= (b(c,\nabla p)\nabla w,\nabla\varphi) + (u(c,\nabla p)\cdot\nabla w,\varphi) + \lambda(w,\varphi) - \langle Gw,\varphi\rangle .$$

Letting $w = \xi$ in (2.27) and using (2.10), (2.21), and (2.22) yields

(2.28)
$$(\xi,\psi) \equiv B(\xi,\varphi)$$
$$= B(\xi,\varphi-\chi) , \quad \chi \in M_h .$$

Then using (2.1), (2.10), and (2.26), we see that

(2.29)
$$|(\xi,\psi)| \le K_{10}\|\xi\|_1 \inf_{\chi\in M_h} \|\varphi-\chi\|_1$$
$$\le K_{11}\|\xi\|_1 h^{k+1} \|\varphi\|_{k+2}$$
$$\le K_{12}\|\xi\|_1 h^{k+1} \|\psi\|_k .$$

Thus, by definition and (2.13), we have

(2.30)
$$\|\xi\|_{-k} \le K_{13}h^{k+1}\|\xi\|_1$$
$$\le K_{14}h^{q+k}\|c\|_q , \quad 2 \le q \le r .$$

Next, if $\tilde{\psi} \in H^{k+\frac{1}{2}}(\partial\Omega)$ and $\tilde{\varphi}$ is the solution of

(2.31)
a) $L\tilde{\varphi} = 0 , \quad x \in \Omega ,$
b) $\hat{L}\tilde{\varphi} = \tilde{\psi} , \quad x \in \partial\Omega ,$

then

(2.32) $$\|\tilde{\varphi}\|_{k+2} \le K_7 |\tilde{\psi}|_{k+\frac{1}{2}} .$$

Using the same techniques as above we obtain for $k \ne 0$,

(2.33) $$|\xi|_{-(k+\frac{1}{2})} \le K_{15}h^{k+q}\|c\|_q , \quad 2 \le q \le r .$$

We note that this estimate was obtained for $k = 0$ in [5]. Next, if $\bar{\psi} \in H^k(\Omega)$ and $\bar{\varphi}$ is the solution of

(2.34)
a) $L\bar{\varphi} = \bar{\psi} , \quad x \in \Omega ,$
b) $b(c,\nabla p)\frac{\partial\varphi}{\partial\nu} + u(c,\nabla p)\cdot\nu\varphi - \frac{\partial g}{\partial u}(\tilde{c})\varphi = 0 , \quad x \in \partial\Omega,$

then, as before,

(2.35) $$\|\bar{\varphi}\|_{k+2} \le K_7 \|\bar{\psi}\|_k ,$$

and letting $w = \xi_t$ in the analogue of (2.27), as above we use (2.23) to obtain

(2.36)
$$(\xi_t,\bar{\psi}) = B(\xi_t,\bar{\varphi}) - N(\bar{\varphi}) + N(\bar{\varphi})$$
$$= B(\xi_t,\bar{\varphi}-\chi) - N(\bar{\varphi}-\chi) + N(\bar{\varphi}) , \quad \chi \in M_h .$$

From (2.35), as in (2.29), we obtain

(2.37)
a) $|B(\xi_t,\bar{\varphi}-\chi)| \le K_{16}\|\xi_t\|_1 h^{k+1}\|\bar{\psi}\|_k .$
b) $|N(\bar{\varphi}-\chi)| \le K_{16}\|\xi\|_1 h^{k+1}\|\bar{\psi}\|_k .$

We note that from (2.24) and the smoothness of g and c, we have

(2.38) $$|\alpha_3|_{-(k+\frac{3}{2})} \le K_{17} |\xi|_{-(k+\frac{1}{2})} .$$

Integrating by parts, using (2.18), (2.24), (2.30), (2.33), (2.35), (2.38), and duality, we obtain

$$|N(\bar{\varphi})| = |(\xi, \nabla a_1 \cdot \nabla\bar{\varphi}) + (\xi, a_1 \Delta\bar{\varphi}) - (\xi, a_1 \frac{\partial\bar{\varphi}}{\partial\nu})$$

$$+ (\xi, \nabla \cdot a_2\bar{\varphi}) + (\xi, a_2 \cdot \nabla\bar{\varphi}) - (\xi, a_2 \cdot \nu\bar{\varphi}) + (a_3, \varphi)|$$

$$(2.39) \quad \le K_{18}(\|\xi\|_{-k}\|\bar{\varphi}\|_{k+2} + |\xi|_{-(k+\frac{1}{2})} \left|\frac{\partial\bar{\varphi}}{\partial\nu}\right|_{k+\frac{1}{2}} + |\xi|_{-(k+\frac{1}{2})} |\bar{\varphi}|_{k+\frac{1}{2}}$$

$$+ |a_3|_{-(k+\frac{3}{2})} |\bar{\varphi}|_{k+\frac{3}{2}})$$

$$\le K_{19} (\|\xi\|_{-k} + |\xi|_{-(k+\frac{1}{2})})\|\bar{\varphi}\|_{k+2}$$

$$\le K_{20}\, h^{k+q}\|c\|_q\|\bar{\psi}\|_k \;.$$

Combining (2.13), (2.36), (2.37), and (2.39) we obtain the desired estimate for the last term on the left side of (2.20). //

We shall first consider discrete-time methods for approximating (1.3). Let $\Delta t > 0$, $N = T/\Delta t \in \mathbb{Z}$, and $t^\sigma = \sigma\,\Delta t$, $\sigma \in \mathbb{R}$. Also let $\psi^n \equiv \psi^n(x) \equiv \psi(x,t^n)$, $d_t\psi^n \equiv (\psi^{n+1}-\psi^n)/\Delta t$, and $\psi^{n+\frac{1}{2}} \equiv (\psi^{n+1}+\psi^n)/2$.

We shall first consider a backward difference in time procedure which will have time discretization error $O(\Delta t)$. Denote the approximation of p by $W:\{0 = t_0, t_1, \ldots, t_N = T\} \to \mathcal{N}_h$ and the approximation of c by $Z:\{t_0, t_1, \ldots, t_N\} \to \mathcal{M}_h$. Assuming that W^n and Z^n are known, we determine W^{n+1} and Z^{n+1} as follows:

$$\text{a)} \quad (\phi d_t Z^n, \chi) + (b(Z^n, \nabla W^n)\nabla Z^{n+1}, \nabla\chi) + (u(Z^n, \nabla W^n)\cdot\nabla Z^{n+j}, \chi)$$
$$= (g(t^{n+1}, Z^{n+j}), \chi) \qquad , \chi \in \mathcal{M}_h\,,$$

(2.40)

$$\text{b)} \quad (a(Z^{n+1})\nabla W^{n+1}, \nabla y) = (a(Z^{n+1})\gamma(Z^{n+1})\nabla d, \nabla y) + (g_1(t^{n+1}), y)\,,$$
$$y \in \mathcal{N}_h,$$

where $j = 0$ or 1. We note that the coefficient matrix arising from the algebraic system (2.40) with $j = 0$ is symmetric. However, in many problems, the transport term is large compared to the diffusion term or the boundary term is large and it may be numerically advantageous to use (2.40) with $j = 1$ even though

the coefficient matrix is no longer symmetric. The remainder of this paper will consider the case $j = 0$.

In order to obtain an approximation with discretization error $O((\Delta t)^2)$ in time, we shall use a Crank-Nicolson-Galerkin scheme with extrapolated coefficients. For this method, replace (2.40a) by

$$(2.41) \quad (\phi d_t Z^n, \chi) + (b(E Z^n, \nabla E W^n)\nabla Z^{n+\frac{1}{2}}, \nabla\chi) + (u(E Z^n, \nabla E W^n)\cdot\nabla E Z^n, \chi)$$
$$= (g(t^{n+1}, E Z^n), \chi)\,, \qquad \chi \in \mathcal{M}_h\,.$$

Since W^{n+1} does not appear in (2.40a) (or (2.41)), we can separate (2.40a) and (2.40b) by first solving (2.40a) at time t^{n+1} and using that solution in the coefficients for the solution of (2.40b) at time t^{n+1}. In this way we have uncoupled (2.40a) and (2.40b) and must only solve two separate linear systems. This greatly reduces the size of our problem and, correspondingly, the work needed to obtain a solution. We also note that lagging the coefficients in (2.40a) and extrapolating them in (2.41) will yield systems of linear equations to solve instead of nonlinear equations.

In the physical problem which motivates our consideration of (1.3), the pressure p is much smoother in time than the concentration c. Thus, in practice, one should use different time steps for the different equations, (2.40a) and (2.40b), and not solve (2.40b) for W at each time step. An analysis of this procedure for the case of (1.3) with homogeneous Neumann conditions appears in [11].

For the nonlinear parabolic problem (1.5), we shall consider the following extrapolated Crank-Nicolson-Galerkin scheme:

$$(2.42) \quad (\phi d_t Z^n, \chi) + (b(E Z^n)\nabla Z^{n+\frac{1}{2}}, \nabla\chi) + (u(E Z^n)\cdot\nabla E Z^n, \chi) = (g(E Z^n), \chi)\,, \quad \chi \in \mathcal{M}_h\,.$$

The time-discretization error for (2.42) is $O((\Delta t)^2)$. Douglas and Dupont analyzed a linear parabolic problem in [5] using extrapolations of the form $2C^{n-\frac{1}{2}} - C^{n-\frac{3}{2}}$ which involved storing the values of C for three previous time levels. In [16], Luskin analyzed a nonlinear parabolic problem using $EC^n = \frac{3}{2}C^n - \frac{1}{2}C^n$ as above. We shall relax the somewhat stringent computational starting condition from [16] while presenting a computationally efficient preconditioned iterative time-stepping procedure.

3. Iterative Stabilization Procedures

In this section, we shall present the linear equations arising from (2.40) (or (2.41)). We note that the coefficient matrices change with each time step. In order to avoid factorization of different matrices at each time step for the solution of the linear equations, we shall discuss an iterative method for approximating their solution. The analysis presented here will extend the results of [6] for a single parabolic equation and [11] for coupled systems to the case of nonlinear boundary contitions.

Let $\{\nu_i\}_{i=1}^{M_1}$ be a basis for M_h and $\{\psi_i\}_{i=1}^{M_2}$ be a basis for N_h. Let Z^m and W^m from (2.40) be written as

(3.1) $$Z^m = \sum_{i=1}^{M_1} \zeta_i^m \nu_i \quad \text{and} \quad W^m = \sum_{i=1}^{M_2} \omega_i^m \psi_i .$$

Using (3.1), (2.40) can be written as

(3.2)
$$\text{a)} \quad L^n(\zeta,\omega)(\zeta^{n+1} - \zeta^n) = \Delta t\, B^n(\zeta,\omega) , \qquad n \geq 1 ,$$
$$\text{b)} \quad A^n(\zeta)\omega^n = \Gamma^n(\zeta) , \qquad n \geq 1 ,$$

where the matrices and vectors are of the form

(3.3)
$$\text{a)} \quad L^n(\zeta,\omega) = ((\phi\nu_j,\nu_i) + \Delta t(b(Z^n,\nabla W^n)\nabla\nu_j,\nabla\nu_i)) ,$$
$$\text{b)} \quad B^n(\zeta,\omega) = (-(b(Z^n,\nabla W^n)\nabla\nu_j,\nabla\nu_i)\zeta^n + (u(Z^n,\nabla W^n)\cdot\nabla\nu_j,\nu_i)\zeta^n + (g(t^{n+1},Z^n),\nu_i)) ,$$
$$\text{c)} \quad A^n(\zeta) = ((a(Z^n)\nabla\psi_\beta,\nabla\psi_\alpha)) ,$$
$$\text{d)} \quad \Gamma^n(\zeta) = ((a(Z^n)\gamma(Z^n)\nabla d,\nabla\psi_\alpha) + (q_1(t^{n+1}),\psi_\alpha)) ,$$

for $i,j = 1,\dots,M_1$ and $\alpha,\beta = 1,\dots,M_2$.

Note that since the matrices L^n and A^n change with time, straightforward solution of (3.2) would involve the factorization of new matrices at each time step. Instead of solving (3.2) exactly, we shall approximate the solution by using an iterative procedure which has been preconditioned by L^0 (or A^0), the associated matrix with coefficients evaluated at $t = 0$, for each time step. The preconditioning process eliminates the need for factoring new matrices at

each time step, while the iterative procedure stabilizes the resulting problem. The stabilization process requires iteration only until a predetermined norm reduction is achieved.

Denote by

(3.4) $$C^m = \sum_{i=1}^{M_1} \alpha_i^m \nu_i \quad \text{and} \quad P^m = \sum_{i=1}^{M_2} \beta_i^m \psi_i$$

the approximations to Z^m and W^m respectively, produced by only approximately solving (3.2). A starting procedure for obtaining C^0, P^0, C^1, and P^1 will be discussed later. Assuming that these quantities are known, we shall find α^{n+1} (and thus C^{n+1}), $n \geq 1$, using a preconditioned iterative method to approximate ζ^{n+1} from (3.2.a). As an initial guess for $\zeta^{n+1} - \zeta^n$ for $n \geq 1$, we shall use linear extrapolation. Specifically, we shall use

(3.5) $$X_0 = \alpha^n - \alpha^{n-1}$$

as the initialization for our iterative procedure for $\alpha^{n+1} - \alpha^n$. Similarly, in order to use linear extrapolation to approximate the solution of (3.2.b), we shall use

(3.6) $$\tilde{X}_0 = 2\beta^n - \beta^{n-1}$$

as an initialization for the iterative procedure for β^{n+1}. Since we then use $\alpha^{n-1}, \alpha^n, \beta^{n-1}$, and β^n in the coefficient matrices to determine α^{n+1}, our errors accumulate.

In order to estimate the cumulative error we first consider the single step error. We define $\bar{\alpha}^{n+1}$ to satisfy

(3.7) $$L^n(\alpha,\beta)(\bar{\alpha}^{n+1} - \alpha^n) = \Delta t\, B^n(\alpha,\beta) , \quad n \geq 1.$$

Similarly, once α^{n+1} has been determined, define $\bar{\beta}^{n+1}$ to satisfy

(3.8) $$A^{n+1}(\alpha^{n+1})\bar{\beta}^{n+1} = \Gamma^{n+1}(\alpha^{n+1}), \qquad n \geq 1 .$$

We can use any preconditioned iterative method which yields the norm reductions of the form

$$\text{(3.9)}\quad \begin{aligned} &\text{a)}\quad \|L^n(\alpha,\beta)^{\frac{1}{2}}(\bar\alpha^{n+1}-\alpha^{n+1})\|_e \le \rho_1 \|L^n(\alpha,\beta)^{\frac{1}{2}}(\bar\alpha^{n+1}-2\alpha^n+\alpha^{n-1})\|_e ,\\ &\text{b)}\quad \|A^n(\alpha)^{\frac{1}{2}}(\bar\beta^{n-1}-\beta^{n+1})\|_e \le \rho_2 \|A^n(\alpha)^{\frac{1}{2}}(\bar\beta^{n+1}-2\beta^n+\beta^{n-1})\|_e \end{aligned}$$

where $0 < \rho_1 < 1$ and $0 < \rho_2 < 1$ and the subscript e indicates the Euclidean norm of the vector. A specific iterative procedure for obtaining (3.9) is the preconditioned conjugate gradient method presented for similar problems in [6,10] and analyzed in [1, 2, 9]. For the preconditioned conjugate gradient method, since the preconditioner is the matrix at time $t = 0$, we have

$$\text{(3.10)}\qquad \rho_1 \le \min\{2\varrho^{\kappa_1}, n\Delta t\}$$

where

$$\text{(3.11)}\qquad \varrho_1 = \frac{1-(\bar\psi_0/\bar\psi_1)^{\frac{1}{2}}}{1+(\bar\psi_0/\bar\psi_1)^{\frac{1}{2}}} ,$$

$\bar\psi_0$ and $\bar\psi_1$ are the comparability constants between the preconditioner L^0 and the matrix L^n given by

$$\text{(3.12)}\qquad 0 < \bar\psi_0 \le \frac{\chi^T L^n(\alpha,\beta)\chi}{\chi^T L^0 \chi} \le \bar\psi_1 \quad , \quad 0 \ne \chi \in \mathbb{R}^{M_1} ,$$

and κ_1 is the number of iterations performed. We note that $\bar\psi_0$ and $\bar\psi_1$ are independent of h and depend only upon the bounds on the coefficients in the problem. Note that for any estimate of the form (3.10), if

$$\text{(3.13)}\qquad \kappa_1 \ge \bar\alpha \log\frac{1}{\Delta t} \Big/ \log\frac{1}{\varrho_1} ,$$

then

$$\text{(3.14)}\qquad \rho_1 < 2(\Delta t)^{\bar\alpha} .$$

Similar estimates hold for the iterative procedure for β^{n+1}.

Let

$$\text{(3.15)}\quad \begin{aligned} &\text{a)}\quad \|\psi\|_\phi^2 \equiv (\phi\psi,\psi),\\ &\text{b)}\quad \|\psi\|_{b^n}^2 \equiv (b(C^n,E\nabla P^n)\nabla\psi,\nabla\psi),\\ &\text{c)}\quad \|\psi\|_{a^n}^2 \equiv (a(C^n)\nabla\psi,\nabla\psi),\\ &\text{d)}\quad |||\psi|||_n \equiv \|\psi\|_\phi + (\Delta t)^{\frac{1}{2}}\|\psi\|_{b^n} , \end{aligned}$$

be special norms and seminorms. Note that $\|\cdot\|_\phi$ is equivalent to $\|\cdot\|$ and $\|\cdot\|_{a^n}$ and $\|\cdot\|_{b^n}$ are uniformly equivalent to $\|\nabla\cdot\|$. Then from (3.7), (3.8), and (3.9)

$$\text{(3.16)}\qquad \bar C^n = \sum_{i=1}^{M_1} \bar\eta_i^n v_i \quad\text{and}\quad \bar P^n = \sum_{i=1}^{M_2} \bar\pi_i^n \psi_i$$

satisfy, for $n \ge 1$,

$$\text{(3.17)}\quad \begin{aligned} &\text{a)}\quad \left(\phi\frac{\bar C^{n+1}-C^n}{\Delta t},\chi\right) + (b(C^n,\nabla P^n)\nabla\bar C^{n+1},\nabla\chi) + (u(C^n,\nabla P^n)\cdot\nabla C^n,\chi)\\ &\qquad = (g(t^{n+1},C^n),\chi), \quad \chi \in M_h ,\\ &\text{b)}\quad (a(C^{n+1})\nabla\bar P^{n+1},\nabla y) = (a(C^{n+1})\gamma(C^{n+1})\nabla d,\nabla y) + (q_1(t^{n+1}),y) , \quad y \in N_h , \end{aligned}$$

and

$$\text{(3.18)}\quad \begin{aligned} &\text{a)}\quad |||\bar C^{n+1}-C^{n+1}|||_n \le \rho_1' \, |||\delta^2 C^n|||_n\\ &\text{b)}\quad \|\bar P^{n+1}-P^{n+1}\|_{a^n} \le \rho_2\|\delta P^n\|_{a^n} + \rho_2\|\bar P^{n+1}-P^{n+1}\|_{a^n} \end{aligned}$$

where we define

$$\text{(3.19)}\quad \begin{aligned} &\text{a)}\quad \delta\psi^n \equiv \psi^{n+1}-\psi^n ,\\ &\text{b)}\quad \delta^2\psi^n \equiv \psi^{n+1}-2\psi^n+\psi^{n-1} ,\\ &\text{c)}\quad \rho_1' = \frac{\rho_1}{1-\rho_1} . \end{aligned}$$

We shall now discuss a starting procedure for obtaining C^0, P^0, C^1 and P^1 which uses the preconditioned iteration described above. At $t = 0$, we shall need a good approximation to the elliptic projection $\tilde c^0$ defined in (2.12). From (2.10) and (2.11) we see that L^0 is comparable to the matrix generated by the form $B(\cdot,\cdot)$ in the definition of $\tilde c$. Thus the same L^0 used for the rest of the iteration will serve as a good preconditioner for the iterative computation of an approximation to $\tilde c^0$ in exactly the right norm. Similarly the iteration defined above with initialization set equal to zero will give a good approximation to $\tilde c^1$ after $O(\log\frac{1}{\Delta t})$ iterations. We thus obtain C^0 (and thus P^0) and C^1 (and P^1) satisfying

$$(3.20)\quad \begin{aligned} &\text{a)} \quad |||C^0-c^0|||_0 + \|\nabla(P-p)^0\| \le K\Delta t \\ &\text{b)} \quad |||C^1-c^1|||_0 + \|\nabla(P-p)^1\| \le K(\Delta t+h^r). \end{aligned}$$

In the case where (2.41) or (2.42) is used we shall need to define a predictor-corrector procedure to retain the same bounds at time $t = \Delta t$ with Δt in (3.20.b) replaced by $(\Delta t)^2$. See [6, 16] for such predictor-corrector starting procedures.

4. A Priori Error Estimates

In this section we develop a priori bounds for the errors $c-C$ and $\nabla(p-P)$ for the problem (1.3) (with $f_1 \equiv 0$) and the iterative procedures defined in Section 3. We obtain $O(\Delta t)$ or $O((\Delta t)^2)$ time-truncation errors depending on whether C is basically defined by (2.40.a) or by (2.41) (or (2.42)) respectively. A fixed number of iterations for solving the pressure equations suffices for all the results presented. In Theorem 4.1, we show that if $b = b(x,c,\nabla p)$ then a norm reduction of $O(\Delta t)$ is necessary for the concentration equations to obtain a spatial error of $O(h^r + h^{s-1})$. This is the same spatial error that was obtained in [12] for the continuous time approximations in this case. In Theorem 4.2 we show that if $b = b(x,c)$ and if slightly more smoothness is assumed on $\frac{\partial c}{\partial t}$ and $\frac{\partial p}{\partial t}$, then a spatial error of $O(h^r + h^s + h^{r+s-3})$ is obtained with a fixed number of iterations of the concentration equations. If the extra smoothness on $\frac{\partial c}{\partial t}$ and $\frac{\partial p}{\partial t}$ is not assumed, $O(\log \frac{1}{h})$ iterations are required for the same estimate. If $b = b(x)$, we show in Theorem 4.4 that, by a simple backsolve at each time step for the concentration equation, a spatial error of $O(h^r + h^s + h^{r+s-3})$ is obtained. Crank-Nicolson-Galerkin methods for higher order time-truncation errors are also briefly discussed.

The special case of a single nonlinear parabolic problem with nonlinear boundary conditions is considered also. Under a mesh restriction assumption which introduces sufficient dissipation into the method, error estimates of $O(h^r + (\Delta t)^2)$ are obtained with a fixed number of iterations per time step in Theorem 4.5.

Theorem 4.1: Assume Ω is H^3-regular (see (2.16)-(2.17)) and (3.20) holds. Let (c,p) satisfy (1.3) with $f_1 \equiv 0$ and (C^n,P^n) satisfy (2.40) (as modified by the iterative procedure of Section 3). If we obtain norm reductions of the form (3.18) with

$$(4.1)\quad \begin{aligned} &\text{a)} \quad \rho_1' \le \Delta t \\ &\text{b)} \quad \rho_2 \le \tfrac{1}{4}(a_*/a^*)^{\frac{1}{2}} , \end{aligned}$$

then there exist positive constants $K_{22} = K_{22}(\lambda, a_*, a^*, b_*, \phi_*, \bar{K}, M; K_i, i=0,\dots,6)$, h_0, and τ_0 such that if $\Delta t \le \tau_0$, and $h \le h_0$,

(4.2) $$\sup_{t^n} \|C-c\| \le K_{22}(h^r + h^{(s-1)} + \Delta t).$$

Proof: Let $\zeta^n = C^n - \tilde{c}^n$ and $\eta^n = P^n - \tilde{p}^n$ and recall that $\xi^n = c^n - \tilde{c}^n$. Subtract (2.7) from (2.40b) to obtain

(4.3)
$$\begin{aligned}(a(C^n)\nabla\eta^n, \nabla y) &= ([a(c^n) - a(C^n)]\nabla\tilde{p}^n, \nabla y)\\ &+ ([a(C^n)\gamma(C^n) - a(c^n)\gamma(c^n)]\nabla d, \nabla y)\\ &+ (a(C^n)\nabla(P^n - \tilde{P}^n), \nabla y), \qquad y \in N_h .\end{aligned}$$

Letting $y = \eta^n$, we can obtain, as in [11],

(4.4) $$\|\eta^n\|_{a^n} \le K_{23}(\|\zeta^n\|_\phi + h^r) + 2\|P^n - \tilde{P}^n\|_{a^n},$$

where $\|\cdot\|_{a^n}$ is defined in (3.15). Next, subtracting (2.12) from (2.40.a), we obtain

(4.5)
$$\begin{aligned}(\phi\, d_t\zeta^n, \chi) &+ (b(C^n, \nabla P^n)\nabla\zeta^{n+1}, \nabla\chi)\\ &= (\phi[\frac{\partial c^{n+1}}{\partial t} - d_t\tilde{c}^n], \chi) - \lambda(\xi^{n+1}, \chi)\\ &+ ([b(c^{n+1}, \nabla p^{n+1}) - b(C^n, \nabla P^n)]\nabla\tilde{c}^{n+1}, \nabla\chi)\\ &+ ([u(c^{n+1}, \nabla p^{n+1})\cdot\nabla\tilde{c}^{n+1} - u(C^n, \nabla P^n)\cdot\nabla C^n], \chi)\\ &+ ([g(t^{n+1}, \tilde{c}^{n+1}) - g(t^{n+1}, C^n)], \chi)\\ &+ (\phi\,\frac{C^{n+1} - \tilde{C}^{n+1}}{\Delta t}, \chi) + (b(C^n, \nabla P^n)\nabla(C^{n+1} - \tilde{C}^{n+1}), \nabla\chi), \qquad \chi \in M_h.\end{aligned}$$

We shall first let $\chi = \zeta^{n+1}$ in (4.5). The left hand side of (4.5) then becomes

(4.6) $$(\phi d_t\zeta^n, \zeta^{n+1}) + (b(C^n, \nabla P^n)\nabla\zeta^{n+1}, \nabla\zeta^{n+1}) = \frac{1}{2\Delta t}(\|\zeta^{n+1}\|_\phi^2 - \|\zeta^n\|_\phi^2) + \|\zeta^{n+1}\|_{b^n}^2 .$$

We shall use Lemmas 2.2 and 2.4 and duality to bound the first two terms on the right of (4.5).

(4.7)
$$\begin{aligned}|(\phi[\frac{\partial c^{n+1}}{\partial t} - d_t\tilde{c}^n], \zeta^{n+1}) - \lambda(\xi^{n+1}, \zeta^{n+1})| &\le K(\|\zeta^{n+1}\|_\phi^2 + \|\xi\|^2 + (\Delta t)^2 + \left\|\frac{\partial\xi^n}{\partial t}\right\|_{-1}\|\zeta^{n+1}\|_1)\\ &\le K_{24}(\|\zeta^{n+1}\|_\phi^2 + (\Delta t)^2 + h^{2r}(\|c^{n+1}\|_r^2 + \left\|\frac{\partial c^n}{\partial t}\right\|_{r-1}^2)) + \frac{1}{8}\|\zeta^{n+1}\|_{b^n}^2 .\end{aligned}$$

For the fourth term on the right of (4.5), we obtain

(4.8)
$$\begin{aligned}&|([u(c^{n+1}, \nabla p^{n+1})\cdot\nabla\tilde{c}^{n+1} - u(C^n, \nabla P^n)\cdot\nabla C^n], \zeta^{n+1})|\\ &\le |([u(c^{n+1}, \nabla p^{n+1}) - u(C^n, \nabla P^n)]\cdot\nabla\tilde{c}^{n+1}, \zeta^{n+1})|\\ &+ |(u(C^n, \nabla P^n)\cdot\nabla[\tilde{c}^{n+1} - \tilde{c}^n - \zeta^n], \zeta^{n+1})|\\ &\le K_{25}(\|\zeta^{n+1}\|_\phi^2 + \|\zeta^n\|_\phi^2 + \|\xi^n\|^2 + \|\eta^n\|_{a^n}^2 + \|\nabla(p-\tilde{p})^n\|^2 + (\Delta t)^2) + \frac{1}{8}\|\zeta^n\|_{b^{n-1}}^2 .\end{aligned}$$

We have used $\|u(C^n, \nabla P^n)\|_{L^\infty} \le K_{26}$ in order to obtain (4.8). From (2.3.f), this amounts to an assumption that $\|\nabla P^n\|_{L^\infty} \le K$. We shall make this more precise with an induction argument. Assume that for h sufficiently small

(I) $$\|\nabla P^n\|_{L^\infty(\Omega)} \le 2K_6 , \quad n = 0,1,\dots,\ell-1.$$

Using (2.2), (2.13), (2.15), (3.20), and (4.4) as in [12], we see that (I) clearly holds for $\ell = 1$. A bound like (4.8) will hold for the third term on the right side of (4.5). By the trace theorem,

(4.9) $$|\psi^{n+1}|^2 \le \bar{K}\,\|\psi^{n+1}\|_\phi \|\psi^{n+1}\|_{b^n} .$$

Using (4.9), we see that

(4.10)
$$\begin{aligned}&|([g(t^{n+1}, \tilde{c}^{n+1}) - g(t^{n+1}, C^n)], \zeta^{n+1})|\\ &\le K_{27}(|\zeta^n| + \Delta t)|\zeta^{n+1}|\\ &\le K_{28}((\Delta t)^2 + \|\zeta^n\|_\phi^2 + \|\zeta^{n+1}\|_\phi^2) + \frac{1}{8}(\|\zeta^n\|_{b^{n-1}}^2 + \|\zeta^{n+1}\|_{b^n}^2) .\end{aligned}$$

From (3.15), (3.18), and (4.4), for $n \ge 1$,

(4.11)
$$\begin{aligned}\|P^n - \tilde{P}^n\|_{a^n} &\le \rho_2(\|P^n - P^{n-1}\|_{a^n} + \|P^n - \tilde{P}^n\|_{a^n})\\ &\le \rho_2(\|\eta^n\|_{a^n} + \left(\frac{a^*}{a_*}\right)^{\frac{1}{2}}\|\eta^{n-1}\|_{a^{n-1}} + \|P^n - \tilde{P}^n\|_{a^n}) + K_{29}\Delta t\\ &\le K_{30}(\|\zeta^n\|_\phi + \|\zeta^{n-1}\|_\phi^2 + h^r + \Delta t) + \rho_2(3\|P^n - \tilde{P}^n\|_{a^n}\\ &\qquad + 2\left(\frac{a^*}{a_*}\right)^{\frac{1}{2}}\|P^{n-1} - \tilde{P}^{n-1}\|_{a^{n-1}}) .\end{aligned}$$

If we sum (4.4) on n from 0 to ℓ and use (4.11), we see that, if

(4.12) $\quad \rho_2 \le \frac{1}{4}(a_*/a^*)^{\frac{1}{2}}$,

then

(4.13) $$\sum_{n=0}^{\ell} \|\eta^n\|_{a^n}^2 \Delta t \le K_3\{\sum_{n=0}^{\ell} \|\zeta^n\|_{\phi}^2 \Delta t + h^{2r} + (\Delta t)^2\} .$$

Next, using (3.15) and (3.18), we obtain

(4.14) $$\begin{aligned}\Big|\Big(\phi\, \frac{C^{n+1}-\bar{C}^{n+1}}{\Delta t}, \zeta^{n+1}\Big) + (b(C^n,\nabla P^n)\nabla(C^{n+1}-\bar{C}^{n+1}),\nabla\zeta^{n+1})\Big| &\le \frac{1}{\Delta t}|||C^{n+1}-\bar{C}^{n+1}|||_n\, |||\zeta^{n+1}|||_n \\ &\le \frac{\rho_1'}{\Delta t}|||\delta^2 C^n|||_n\, |||\zeta^{n+1}|||_n \\ &\le \frac{1}{8}\|\zeta^{n+1}\|_{b^n}^2 + K_{32}\|\zeta^{n+1}\|_{\phi}^2 + \frac{\rho_1'^2\epsilon_1}{(\Delta t)^2}\{|||\delta\zeta^n|||_n^2 + |||\delta\zeta^{n-1}|||_{n-1}^2\} \\ &\quad + (\Delta t)^2 .\end{aligned}$$

If we iterate κ_1 times, where κ_1 satisfies (3.13) with $\tilde{\alpha} = 1$, we see that

(4.15) $$\begin{aligned}\frac{\rho_1'^2\epsilon_1}{(\Delta t)^2}\{|||\delta\zeta^n|||_n^2 + |||\delta\zeta^{n-1}|||_{n-1}^2\} &\le \frac{\Delta t}{8}\{\|\zeta^{n+1}\|_{b^n}^2 + \|\zeta^n\|_{b^{n-1}}^2 + \|\zeta^{n-1}\|_{b^{n-2}}^2\} \\ &\quad + K_{33}\{\|\zeta^{n+1}\|_{\phi}^2 + \|\zeta^n\|_{\phi}^2 + \|\zeta^{n-1}\|_{\phi}^2\}.\end{aligned}$$

We next multiply (4.5) by Δt, sum on n from 0 to $\ell-1$, use Lemmas 2.1 and (2.2), (4.6)-(4.10), (4.13), (4.14), and (4.5) to obtain

(4.16) $$\frac{1}{2}\|\zeta^\ell\|_{\phi}^2 \le K_{34}\{\sum_{n=0}^{\ell} \|\zeta^n\|_{\phi}^2 \Delta t + \|\zeta^0\|_{\phi}^2 + \Delta t\|\nabla\zeta^0\|^2 + h^{2r} + h^{2(s-1)} + (\Delta t)^2\} .$$

Then an application of the discrete Gronwall's Lemma and (3.20) yield the desired result. We then use (2.2), (2.13), (2.15), and (4.4) as in [12] to see that for h sufficiently small, our induction hypothesis (I) is satisfied for $n = \ell$. //

We note that the need to iterate sufficiently often to make the norm reduction (3.9.a) of the size $O(\Delta t)$, comes from the fact that we were not able to make use of the differences in the terms on the left of (4.15). This difference can often be estimated by using the test function $\chi = \zeta^{n+1}-\zeta^n = \Delta t d_t\zeta^n$ in (4.5).

It was noted in [11] that in the case $b = b(x,c,\nabla p)$ the standard trick of summation by parts in time to estimate the third term on the right of (4.5) with the new test function will not work unless c and ∇p are tied together in a special way. In the physical problem under consideration, $b = b(x,u)$ where u is defined in (1.1.a). Mixed methods for solving the pressure equation using a system of first order problems in the variables p and u have just been analyzed [7]. Efficient time-stepping methods for systems utilizing mixed methods will appear elsewhere.

In the case $b = b(x,c)$ (considered in [12]), we can make use of the differences in (4.15) and obtain better results than those in Theorem 4.1. We shall first assume slightly more smoothness on c. We assume that $\frac{\partial c}{\partial t} \in L^2(J;H^r)$. We shall also use an idea from [3] to require less restrictive assumptions on the starting procedure than is required in [6, 11, 16].

<u>Theorem 4.2.</u> Let (c,p) satisfy (1.3) (with $f_1 \equiv 0$ and $b = b(x,c)$) and (C^n,P^n) satisfy the iterative modification of (2.40). Assume (3.20) is satisfied and $\frac{\partial c}{\partial t} \in L^2(J;H^r)$ and $\frac{\partial p}{\partial t} \in L^2(J;H^s)$. If we obtain norm reductions of the form (3.18) with

(4.17)
a) $\rho_1' \le \frac{1}{4}(1 + 2\frac{b^*}{b_*})^{-1}$,

b) $\rho_2 \le \frac{1}{4}(a_*/a^*)^{\frac{1}{2}}$,

then there exist positive constants $K_{35} = K_{35}(\lambda,a_*,a^*,b_*,\phi_*,\bar{K},M;K_i,i=0,\ldots,6)$, h_0, and τ_0 such that if $\Delta t \le \tau_0$ and $h \le h_0$,

(4.18) $$\sup_{t^n} \|C-c\| \le K_{35}\{h^r + h^s + h^{r+s-3} + \Delta t\} .$$

<u>Proof:</u> As in the proof of Theorem 4.1, we shall without loss of generality assume that

(4.19) $$\|\nabla P\|_{L^\infty(J;L^\infty)} \le 2K_6 ,$$

since we can obtain L^∞ estimates from (4.18) and (4.4).

We first use $\chi = \zeta^{n+1}$ as a test function in the modified (4.5). We shall need to obtain an improved estimate for (4.8). Recalling that $u(x,c,\nabla p) = -a(c)[\nabla p-\gamma(c)\nabla d]$, we note that

$$|([u(c^{n+1},\nabla p^{n+1}) - u(c^{n+1},\nabla\tilde{p}^{n+1}) + u(c^{n+1},\nabla\tilde{p}^{n+1})-u(C^n,\nabla P^n)]\cdot\nabla\tilde{c}^{n+1},\zeta^{n+1})|$$

$$\le |(a(c^{n+1})\nabla(p-\tilde{p})^{n+1}\cdot\nabla\tilde{c}^{n+1},\zeta^{n+1})| + |([u(c^{n+1},\nabla\tilde{p}^{n+1})-u(C^n,\nabla P^n)]\cdot\nabla\tilde{c}^{n+1},\zeta^{n+1})|$$

$$\le |((p-\tilde{p})^{n+1},\nabla\cdot(a(c^{n+1})\zeta^{n+1}\nabla\tilde{c}^{n+1}))| + |\langle(p-\tilde{p})^{n+1},a(c^{n+1})\zeta^{n+1}\nabla\tilde{c}^{n+1}\cdot\nu\rangle| \qquad (4.20)$$

$$+ K_{36}\{\|\zeta^{n+1}\|_\phi^2 + \|\zeta^n\|_\phi^2 + \|\xi^n\|^2 + (\Delta t)^2 + \|\eta^n\|_{a^n}^2\}$$

$$\le K_{37}\{\|\zeta^{n+1}\|_\phi^2 + \|\zeta^n\|_\phi^2 + \|\xi^n\|^2 + \|\eta^n\|_{a^n}^2 + (\Delta t)^2 + \|(p-\tilde{p})^{n+1}\|^2\} + \frac{1}{8}\|\zeta^{n+1}\|_{b^n}^2$$

$$+ |\langle(p-\tilde{p})^{n+1},a(c^{n+1})\zeta^{n+1}\nabla\tilde{c}^{n+1}\cdot\nu\rangle| .$$

Using a Nitsche lift [17] as in [11,12], we can obtain

$$|\langle(p-\tilde{p})^{n+1},a(c^{n+1})\zeta^{n+1}(\nabla(\tilde{c}-c)^{n+1} + \nabla c^{n+1})\cdot\nu\rangle|$$
$$\le \frac{1}{8}\|\zeta^{n+1}\|_{b^n}^2 + K_{38}\{h^{2s} + h^{2r+2s-6}\} . \qquad (4.21)$$

Combining (4.20) and (4.21) with the other estimates for (4.5) obtained in the proof of Theorem 4.1, we see that for some $\varepsilon_1 > 0$ (to be chosen later),

$$\frac{1}{2}\{\|\zeta^\ell\|_\phi^2 + \sum_{n=1}^{\ell-1}\|\zeta^{n+1}\|_{b^n}^2\,\Delta t\} \le K_{39}\{\sum_{n=0}^{\ell}\|\zeta^n\|_\phi^2\,\Delta t + |||\,\zeta^0\,|||_0^2 \qquad (4.22)$$

$$+ h^{2r+2s-6} + h^{2r} + h^{2s} + (\Delta t)^2\} + \frac{\rho_1^2\varepsilon_1}{\Delta t}\sum_{n=0}^{\ell-1}|||\delta\zeta^n|||_n^2 .$$

In order to try to obtain a bound for the last term on the right of (4.15), we shall use the test function $\chi = \zeta^{n+1}-\zeta^n = \delta\zeta^n$ in (4.5). In order to make as weak assumptions on c^0 as possible, we shall use a technique from [3]. Multiply the equation (4.5) for $t = t^n$ by $n\Delta t = t^n \le T$ to obtain a modified (4.5) for $n=1,\dots,\ell-1$. After a slight rearrangement, the left side of the modified (4.5) then becomes

$$n\Delta t\{\frac{1}{\Delta t}\|\delta\zeta^n\|_\phi^2 + \frac{1}{2}(b(C^n)\nabla(\zeta^{n+1}-\zeta^n),\delta\zeta^n) + \frac{1}{2}(b(C^n)\nabla(\zeta^{n+1}+\zeta^n),\delta\zeta^n)\}$$

$$= n\{\|\delta\zeta^n\|_\phi^2 + \frac{\Delta t}{2}\|\delta\zeta^n\|_{b^n}^2\} + \frac{n\Delta t}{2}\{\|\zeta^{n+1}\|_{b^n}^2 - \|\zeta^n\|_{b^n}^2\} \qquad (4.23)$$

$$\ge \frac{n}{2}\{\|\delta\zeta^n\|_\phi^2 + |||\delta\zeta^n|||_n^2\} + \frac{n\Delta t}{2}\{\|\zeta^{n+1}\|_{b^n}^2 - \|\zeta^n\|_{b^n}^2\} .$$

Using the fact that $n\Delta t = T$, the first two terms on the right of the modified (4.5) are bounded as follows

$$n\Delta t|(\phi[\frac{\partial c^{n+1}}{\partial t} - d_t\tilde{c}^n],\delta\zeta^n) - \lambda(\xi^{n+1},\delta\zeta^n)|$$

$$\le K_{40}\Delta t\{\|\xi^{n+1}\|^2 + \left\|\frac{\partial\xi^n}{\partial t}\right\|^2 + (\Delta t)^2\} + \frac{n}{16}\|\delta\zeta^n\|_\phi^2 \qquad (4.24)$$

$$\le K_{40}\,\Delta t\{K_4^2h^{2r}[\|c^{n+1}\|_r + \|\frac{\partial c^n}{\partial t}\|_r]^2 + (\Delta t)^2\} + \frac{n}{16}\|\delta\zeta^n\|_\phi .$$

Summing the fourth term of the right of the modified (4.5) on n, we use the form of u to obtain

$$\sum_{n=1}^{\ell-1} n\Delta t([u(c^{n+1},\nabla p^{n+1})\cdot\nabla\tilde{c}^{n+1}-u(C^n,\nabla P^n)\cdot\nabla C^n],\delta\zeta^n)|$$

$$= \sum_{n=1}^{\ell-1} n\,\Delta t(a(c^{n+1})\nabla(p-\tilde{p})^{n+1}\cdot\nabla\tilde{c}^{n+1},\delta\zeta^n) \qquad (4.25)$$

$$+ \sum_{n=1}^{\ell-1} n\Delta t([u(c^{n+1},\nabla\tilde{p}^{n+1}) - u(C^n,\nabla P^n)]\cdot\nabla\tilde{c}^{n+1}+u(C^n,\nabla P^n)\cdot\nabla[\tilde{c}^{n+1}-C^n],\delta\zeta^n)$$

$$\equiv T_1 + T_2 .$$

As before, we see that

$$|T_2| \le \sum_{n=1}^{\ell-1}\frac{n}{16}\|\delta\zeta^n\|_\phi^2 + K_{41}\sum_{n=1}^{\ell-1}\{\|\zeta^n\|_{b^{n-1}}^2 n\Delta t + \|\xi^n\|^2 + \|\eta^n\|_{a^n}^2 + \|\zeta^n\|_\phi^2 + (\Delta t)^2\}\Delta t. \qquad (4.26)$$

Summing by parts in time and denoting $a^{n+1} = a(c^{n+1})$, we obtain

$$|T_1| \le \Big| \sum_{n=1}^{\ell-1} (n\Delta t a^{n+1}\nabla(p-\bar p)^{n+1}\cdot\nabla\bar c^{n+1} - (n-1)\Delta t a^{n}\nabla(p-\bar p)^{n}\cdot\nabla\bar c^{n}, \zeta^n)\Big|$$

$$+ \big|((\ell-1)\Delta t a^{\ell}\nabla(p-\bar p)^{\ell}\cdot\nabla\bar c^{\ell}, \zeta^{\ell})\big| + \big|(\Delta t a^{2}\nabla(p-\bar p)^{2}\cdot\nabla\bar c^{2}, \zeta^{1})\big|$$

(4.27)

$$\le \Big| \sum_{n=1}^{\ell-1} (n\Delta t a^{n+1}\nabla(p-\bar p)^{n+1}\cdot\nabla d_t\bar c^{n}, \zeta^n)\Delta t\Big|$$

$$+ \Big| \sum_{n=1}^{\ell-1} (n\Delta t a^{n+1}\nabla d_t(p-\bar p)^{n}\cdot\nabla\bar c^{n}, \zeta^n)\Delta t\Big|$$

$$+ \Big| \sum_{n=1}^{\ell-1} (n\Delta t \frac{\partial a}{\partial c} d_t c^n\nabla(p-\bar p)^{n}\cdot\nabla\bar c^{n}, \zeta^n)\Delta t\Big|$$

$$+ \Big| \sum_{n=1}^{\ell-1} (a^n\nabla(p-\bar p)^{n}\cdot\nabla\bar c^{n}, \zeta^n)\Delta t\Big|$$

$$+ \big|((\ell-1)\Delta t a^{\ell}\nabla(p-\bar p)^{\ell}\cdot\nabla\bar c^{\ell}, \zeta^{\ell})\big| + \big|(a^{2}\nabla(p-\bar p)^{2}\cdot\nabla\bar c^{2}, \zeta^{1}\Delta t)\big|$$

$$\equiv T_3 + T_4 + T_5 + T_6 + T_7 + T_8 .$$

We note that

(4.28)

$$T_3 \le \Big| \sum_{n=1}^{\ell-1} (n\Delta t a^{n+1}\nabla(p-\bar p)^{n+1}\cdot\nabla d_t(\bar c-c)^{n}, \zeta^n)\Delta t\Big|$$

$$+ \Big| \sum_{n=1}^{\ell-1} (n\Delta t a^{n+1}\nabla(p-\bar p)^{n+1}\cdot\nabla d_t c^{n}, \zeta^n)\Delta t\Big|$$

$$\equiv T_9 + T_{10}.$$

Using (2.2) and Lemmas 2.1 and 2.2, we obtain

(4.29)

$$T_9 \le \sum_{n=1}^{\ell-1} K_{42}\|\nabla(p-\bar p)^{n+1}\|\,\|\nabla d_t(\bar c-c)^n\|\,\|\zeta^n\|_{L^\infty}\Delta t$$

$$\le \sum_{n=1}^{\ell-1} K_{43}\, h^{r+s-3}\|\zeta^n\|_{\phi}\Delta t$$

$$\le K_{44}\{ \sum_{n=1}^{\ell-1} \|\zeta^n\|_{\phi}^2\, \Delta t + h^{2r+2s-6}\} .$$

We integrate by parts to bound T_{10}. As in (4.21), we have

(4.30)

$$T_{10} \le \Big| \sum_{n=1}^{\ell-1} n\Delta t((p-\bar p)^{n+1}, \nabla\cdot[a^{n+1}\zeta^n\nabla d_t c^n])\Delta t\Big|$$

$$+ \Big| \sum_{n=1}^{\ell-1} n\Delta t\,((p-\bar p)^{n+1}, a^{n+1}\zeta^n\nabla d_t c^n\cdot \nu)\Delta t\Big|$$

$$\le K_{45}\{ \sum_{n=1}^{\ell-1} n\Delta t\,\|\zeta^n\|_{b^{n-1}}^2\,\Delta t + h^{2s}\}.$$

Using the same techniques as above we see that

(4.31)

$$T_4 + T_5 + T_6 + T_7 + T_8 \le K_{46}\{ \sum_{n=1}^{\ell} [\|\zeta^n\|_{\phi}^2 + \|\zeta^n\|_{b^{n-1}}^2\, n\Delta t]\Delta t$$

$$+ h^{2s} + h^{2r+2s-6}\} + \frac{1}{16}\{\|\zeta^{\ell}\|_{\phi}^2 + \|\zeta^{\ell}\|_{b^{\ell-1}}^2\}\,\ell\Delta t$$

$$+ \frac{1}{16}\sum_{n=1}^{\ell-1}\|\zeta^n\|_{b^{n-1}}^2\,\Delta t .$$

We note that the last term on the right of (4.31) came from T_6 .

In order to bound the third term on the right of the modified (4.5), we shall first sum by parts in time.

(4.32)

$$\Big|\sum_{n=1}^{\ell-1} ([b(c^{n+1})-b(c^n)]\nabla\bar c^{n+1}, \nabla(\zeta^{n+1} - \zeta^n))n\Delta t\Big|$$

$$\le \Big|\sum_{n=2}^{\ell-1} ([\{b(c^{n+1})-b(c^n)\}\nabla\bar c^{n+1} n\Delta t - \{b(c^n)-b(c^{n-1})\}\nabla\bar c^{n}(n-1)\Delta t], \nabla\zeta^n)\Big|$$

$$+ \{\big|([b(c^{\ell}) - b(c^{\ell-1})]\nabla\bar c^{\ell}(\ell-1)\Delta t, \nabla\zeta^{\ell})\big| + \big|([b(c^2)-b(c^1)]\nabla\bar c^{2}\Delta t, \nabla\zeta^1)\big|\}$$

$$\equiv T_{11} + T_{12} .$$

Note that

(4.33)

$$T_{12} \le \frac{1}{16}\{\ell\Delta t\|\zeta^{\ell}\|_{b^{\ell-1}}^2 + \Delta t\|\zeta^1\|_{b^0}^2\}$$

$$+ K_{47}\{(\ell-1)\Delta t\,\|\zeta^{\ell-1}\|_{\phi}^2 + (\Delta t)\|\zeta^1\|_{\phi}^2 + h^{2r} + (\Delta t)^2\} .$$

Next, we see that

$$T_{11} \le \Big| \sum_{n=2}^{\ell-1} ([b(c^n) - b(C^{n-1})]\nabla[n\bar{c}^{n+1} - (n-1)\bar{c}^n]\Delta t, \nabla\zeta^n)\Big|$$

(4.34) $$+ \Big| \sum_{n=2}^{\ell-1} ([b(c^{n+1}) - b(C^n) - \{b(c^n) - b(C^{n-1})\}]\cdot\nabla\bar{c}^{n+1} n\Delta t, \nabla\zeta^n)\Big|$$

$$\equiv T_{13} + T_{14}.$$

For T_{13}, we obtain

(4.35) $$T_{13} \le K_{48}\Big\{\sum_{n=1}^{\ell-1} [\|\zeta^n\|^2_{b^{n-1}} n\Delta t + \|\zeta^n\|^2_\phi]\Delta t + h^{2r} + (\Delta t)^2\Big\} + \frac{1}{16}\sum_{n=2}^{\ell-1} \|\zeta^n\|^2_{b^{n-1}}\Delta t.$$

Next define

(4.36)
a) $$b'_{1,n}(x) = \int_0^1 \frac{\partial b}{\partial c}(x, \theta c^{n+1} + (1-\theta)c^n)d\theta,$$

b) $$b'_{2,n}(x) = \int_0^1 \frac{\partial b}{\partial c}(x, \theta C^n + (1-\theta)C^{n-1})d\theta.$$

Then we see that

$$T_{14} = \Big| \sum_{n=2}^{\ell-1} (b'_{1,n}\,\delta c^n - b'_{2,n}\,\delta C^{n-1})\cdot\nabla\bar{c}^{n+1} n\Delta t, \nabla\zeta^n)\Big|$$

$$= \Big| \sum_{n=2}^{\ell-1} ([\{b'_{1,n} - b'_{2,n}\}d_t c^n \Delta t$$

(4.37) $$+ b'_{2,n}\{d_t^2 c^n(\Delta t)^2 + \delta\zeta^n\}]\cdot\nabla\bar{c}^{n+1} n\Delta t, \nabla\zeta^n)\Big|$$

$$\le K_{49}\Big\{\sum_{n=1}^{\ell-1} [\|\zeta^n\|^2_{b^{n-1}} n\Delta t + \|\zeta^n\|^2_\phi]\Delta t + h^{2r} + (\Delta t)^2\Big\}$$

$$+ \sum_{n=2}^{\ell-1} \frac{1}{16}\|\delta\zeta^n\|^2_\phi.$$

Next we consider the fifth term on the right of (4.5)

$$\Big|\sum_{n=1}^{\ell-1}(g(\bar{c}^{n+1}) - g(C^n), \delta\zeta^n) n\Delta t\Big| \le \Big|\sum_{n=1}^{\ell-1}(g(\bar{c}^{n+1}) - g(\bar{c}^n), \delta\zeta^n) n\Delta t\Big|$$

(4.38) $$+ \Big|\sum_{n=1}^{\ell-1}(g(\bar{c}^n) - g(C^n), \delta\zeta^n) n\Delta t\Big|$$

$$\equiv T_{15} + T_{16}.$$

Define

(4.39)
a) $$g'_{1,n}(x) = \int_0^1 \frac{\partial g}{\partial c}(x, t^{n+1}, \theta\bar{c}^{n+1} + (1-\theta)\bar{c}^n)d\theta,$$

b) $$g'_{2,n}(x) = \int_0^1 \frac{\partial g}{\partial c}(x, t^{n+1}, \theta\bar{c}^n + (1-\theta)C^n)d\theta.$$

We see that since $\zeta^n = \frac{1}{2}(\zeta^{n+1} + \zeta^n) - \frac{1}{2}\delta\zeta^n$,

$$T_{16} = \sum_{n=1}^{\ell-1} (g'_{2,n}\zeta^n, \delta\zeta^n)$$

(4.40) $$\le \Big|\sum_{n=1}^{\ell-1}(g'_{2,n}\,\tfrac{1}{2}(\zeta^{n+1}+\zeta^n), \delta\zeta^n) n\Delta t\Big| + \Big|\sum_{n=1}^{\ell-1}(g'_{2,n}\,\tfrac{1}{2}\delta\zeta^n, \delta\zeta^n) n\Delta t\Big|$$

$$\le \Big|\sum_{n=1}^{\ell-1}\tfrac{1}{2}(g'_{2,n}, (\zeta^{n+1})^2 - (\zeta^n)^2) n\Delta t\Big| + \Big|\sum_{n=1}^{\ell-1} K_{50}|\delta\zeta^n|^2 n\Delta t\Big|$$

$$\equiv T_{17} + T_{18}.$$

Summing by parts, we see that

$$T_{17} \le \Big|\sum_{n=2}^{\ell-1}\tfrac{1}{2}(g'_{2,n}\,n - g'_{2,n-1}(n-1), (\zeta^n)^2)\Delta t\Big| + \Big|\tfrac{1}{2}(g'_{2,\ell-1}, (\zeta^\ell)^2)(\ell-1)\Delta t\Big|$$

(4.41) $$+ \Big|\tfrac{1}{2}(g'_{2,1}, (\zeta^1)^2)\Delta t\Big|$$

$$\equiv T_{19} + T_{20} + T_{21}.$$

Then using (4.9) we have

(4.42) $$T_{18} + T_{20} + T_{21} \le \frac{1}{16}\Big(\sum_{n=1}^{\ell-1} n\|\delta\zeta^n\|^2_\phi + \|\zeta^1\|^2_{b^0}\Delta t + \|\zeta^\ell\|^2_{b^{\ell-1}}\ell\Delta t\Big)$$

$$+ K_{51}\Big(\sum_{n=1}^{\ell-1}\|\zeta^n\|^2_{b^{n-1}} n(\Delta t)^2 + \|\zeta^\ell\|^2_\phi\,\ell\Delta t + \|\zeta^1\|^2_\phi\Delta t\Big).$$

Since

(4.43) $$|g'_{2,n} - g'_{2,n-1}| = \Big|\int_0^1 \Big(\frac{\partial^2 g}{\partial t\,\partial c}\Delta t + \frac{\partial^2 g}{\partial c^2}[\theta d_t\bar{c}^{n-1}\Delta t + (1-\theta)\delta\zeta^{n-1}]\Big)d\theta\Big|$$

$$\le K_{52}[\Delta t + \|\delta\zeta^{n-1}\|_{L^\infty}].$$

we have

$$T_{19} \le \Big|\sum_{n=2}^{\ell-1} \frac{1}{2}\, n\Delta t\, (g'_{2,n}-g'_{2,n-1}, (\zeta^n)^2)\Big| + \Big|\sum_{n=2}^{\ell-1} \frac{1}{2} (g'_{2,n-1}, (\zeta^n)^2)\,\Delta t\Big|$$

(4.44)
$$\le \sum_{n=2}^{\ell-1} K_{53}\{[\|\delta\zeta^{n-1}\|_{L^\infty} + \Delta t]\|\zeta^n\|_\phi \|\zeta^n\|_{b^{n-1}} n\Delta t + \|\zeta^n\|_\phi \|\zeta^n\|_{b^{n-1}}\Delta t\}$$

$$\le \frac{1}{16}\sum_{n=2}^{\ell-1}\|\zeta^n\|^2_{b^{n-1}}\Delta t + K_{54}\sum_{n=2}^{\ell-1}\{\|\zeta^n\|^2_{b^{n-1}} n(\Delta t)^2 + [n\|\zeta^{n-1}\|^2_{L^\infty} + \Delta t]\|\zeta^n\|^2_\phi\}.$$

We next bound T_{15}. Summing by parts and using (4.39), we use the above techniques to obtain

$$T_{15} = \Big|\sum_{n=1}^{\ell-1}(g'_{1,n} n d_t \bar{c}^n, \delta\zeta^n)(\Delta t)^2\Big|$$

(4.45)
$$\le \Big|\sum_{n=2}^{\ell-1}(g'_{1,n} n d_t \bar{c}^n - g'_{1,n-1}(n-1)d_t\bar{c}^{n-1}, \zeta^n)(\Delta t)^2\Big|$$

$$+ \ |(g'_{1,\ell-1}(\ell-1)d_t\bar{c}^{\ell-1}, \zeta^\ell)(\Delta t)^2| + |(g'_{1,2}d_t c^1, \zeta^1)(\Delta t)^2|$$

$$\le \frac{1}{16}\{\|\zeta^\ell\|^2_{b^{\ell-1}}\ \ell\Delta t + \sum_{n=1}^{\ell-1}\|\zeta^n\|^2_{b^{n-1}}\Delta t\} + K_{55}\{\sum_{n=1}^{\ell-1}\|\zeta^n\|^2_\phi\,\Delta t + (\Delta t)^2\}.$$

For the last two terms on the right of the modified (4.5) we use (3.15) and (3.18) to obtain

$$\sum_{n=1}^{\ell-1}\Big|\Big(\phi\frac{c^{n+1}-\bar{c}^{n+1}}{\Delta t}, \delta\zeta^n\Big) + (b(c^n)\nabla(c^{n+1}-\bar{c}^{n+1}), \nabla\delta\zeta^n)\Big| n\Delta t$$

$$\le \sum_{n=1}^{\ell-1}\frac{1}{\Delta t}\,|||c^{n+1}-\bar{c}^{n+1}|||_n\,|||\delta\zeta^n|||_n\ n\Delta t$$

(4.46)
$$\le \sum_{n=1}^{\ell-1}\frac{\rho'_1}{\Delta t}\,|||\delta^2 c^n|||_n\,|||\delta\zeta^n|||_n\ n\Delta t$$

$$\le \sum_{n=1}^{\ell-1}\frac{\rho'_1}{\Delta t}\{K_{56}(\Delta t)^2 + |||\delta\zeta^n|||^2_n + |||\delta\zeta^{n-1}|||^2_{n-1}\frac{b^*}{b_*}\}\,|||\delta\zeta^n|||_n\, n\Delta t$$

$$\le \sum_{n=1}^{\ell-1}\frac{n}{4}\,|||\delta\zeta^n|||^2_n + K_{57}(\Delta t)^2.$$

We note that for the last inequality in (4.46) we have chosen

(4.47)
$$\rho'_1 \le \frac{1}{4}\Big(1 + \frac{2b^*}{b_*}\Big)^{-1}.$$

Combining the estimates (4.13), (4.23)-(4.46), we obtain

$$\sum_{n=1}^{\ell-1}\frac{n}{4}\{\|\delta\zeta^n\|^2_\phi + |||\delta\zeta^n|||^2_n\} + \sum_{n=1}^{\ell-1}\frac{1}{2}\{\|\zeta^{n+1}\|^2_{b^n} - \|\zeta^n\|^2_{b^n}\}n\Delta t$$

(4.48)
$$\le \frac{1}{4}\{[\|\zeta^\ell\|^2_\phi + \|\zeta^\ell\|^2_{b^{\ell-1}}]\ell\Delta t + \sum_{n=1}^{\ell-1}\|\zeta^n\|^2_{b^{n-1}}\Delta t\}$$

$$+ K_{58}\{\sum_{n=1}^{\ell-1}[n\|\delta\zeta^{n-1}\|^2_{L^\infty} + \Delta t][\|\zeta^n\|^2_\phi + \|\zeta^n\|^2_{b^{n-1}}\,n\Delta t]$$

$$+ h^{2r} + h^{2s} + h^{2r+2s-6} + (\Delta t)^2 + K_{47}\|\zeta^{\ell-1}\|^2_\phi(\ell-1)\Delta t + K_{51}\|\zeta^\ell\|^2_\phi\ell\Delta t.$$

We next present a technique to introduce terms on the left side of (4.48) to dominate the terms multiplied by K_{47} and K_{51}. Note that

(4.49)
$$n\Delta t(\|\zeta^{n+1}\|^2_\phi - \|\zeta^n\|^2_\phi) = 2n\Delta t(\phi\zeta^n, \delta\zeta^n) + n\Delta t\|\delta\zeta^n\|^2_\phi.$$

Then we have

(4.50)
$$(n+1)\Delta t\|\zeta^{n+1}\|^2_\phi - n\Delta t\|\zeta^n\|^2_\phi - \Delta t\|\zeta^{n+1}\|^2_\phi \le \tfrac{\epsilon}{2} n\|\delta\zeta^n\|^2_\phi + K_{59}\,\Delta t\|\zeta^n\|^2_\phi.$$

We shall sum (4.50) from $n=1$ to upper limits $\ell-1$ and $\ell-2$ and multiply the results by $K_{51}+\frac{1}{2}$ and K_{47} respectively; then we shall add the resulting inequalities to the inequality (4.48). We next want to obtain a telescoping sum from the second term on the left of (4.48).

Note that

$$\|\zeta^n\|^2_{b^n} = \|\zeta^n\|^2_{b^{n-1}} + ([b(c^n) - b(c^{n-1})]\nabla\zeta^n, \nabla\zeta^n)$$

(4.51)
$$= \|\zeta^n\|^2_{b^{n-1}} + \Big(\frac{\partial b}{\partial c}[\delta\zeta^{n-1} + \delta\bar{c}^{n-1}]\nabla\zeta^n, \nabla\zeta^n\Big)$$

$$\le \|\zeta^n\|^2_{b^{n-1}} + K_{60}(\|\delta\zeta^{n-1}\|_{L^\infty} + \Delta t)\|\zeta^n\|^2_{b^{n-1}}.$$

We then see that

$$\sum_{n=0}^{\ell-1} \frac{1}{2}\{\|\zeta^{n+1}\|^2_{b^n} - \|\zeta^n\|^2_{b^n}\}n\Delta t$$

(4.52)

$$\geq \sum_{n=0}^{\ell-1} \frac{1}{2}\{\|\zeta^{n+1}\|^2_{b^n}(n+1)\Delta t - \|\zeta^n\|^2_{b^{n-1}}n\Delta t - \|\zeta^{n+1}\|^2_{b^n}\Delta t$$

$$- K_{60}[\|\delta\zeta^{n-1}\|_{L^\infty} + \Delta t]\|\zeta^n\|^2_{b^{n-1}}n\Delta t\}.$$

Note that the bottom term in the telescoping sum has a zero multiplier and does not contribute anything to the sum. In order to treat the term in (4.52) which is multiplied by K_{60}, we split it in the following way:

$$K_{60}\sum_{n=2}^{\ell-1}\|\delta\zeta^{n-1}\|_{L^\infty}\|\zeta^n\|^2_{b^{n-1}}n\Delta t \leq \frac{1}{16}\sum_{n=2}^{\ell-1}\|\zeta^n\|^2_{b^{n-1}}\Delta t$$

(4.53)

$$+ K_{61}\sum_{n=2}^{\ell-1} n\,\|\delta\zeta^{n-1}\|^2_{L^\infty}\|\zeta^n\|^2_{b^{n-1}}\, n\Delta t.$$

Letting

$$\varepsilon_2 \leq \{8(K_{47} + K_{51} + \tfrac{1}{2})\}^{-1}$$

and combining (4.48)-(4.53), we obtain

$$\sum_{n=0}^{\ell-1}\frac{n}{8}\{\|\delta\zeta^n\|^2_\phi + |||\delta\zeta^n|||^2_n\} + \frac{1}{4}\{\|\zeta^\ell\|^2_\phi + \|\zeta^\ell\|^2_{b^{\ell-1}}\}\ell\Delta t$$

(4.54)

$$\leq K_{62}\{\sum_{n=1}^{\ell-1}[n\|\delta\zeta^{n-1}\|^2_{L^\infty} + \Delta t](\|\zeta^n\|^2_{b^{n-1}}\, n\Delta t + \|\zeta^n\|^2_\phi)$$

$$+ h^{2r} + h^{2s} + h^{2r+2s-6} + (\Delta t)^2\} + \frac{3}{4}\sum_{n=1}^{\ell-1}\|\zeta^{n+1}\|^2_{b^n}\Delta t + |||\zeta^0|||^2_0 .$$

We now want to combine (4.22) and (4.54) in a special way. In order to hide the next to the last term on the right of (4.54) on the left hand side of (4.22), we multiply (4.54) by 1/2, add the result to (4.22) and simplify to obtain

$$\frac{1}{2}\|\zeta^\ell\|^2_\phi + \frac{1}{8}\{\|\zeta^\ell\|^2_\phi + \|\zeta^\ell\|^2_{b^{\ell-1}}\}\ell\Delta t + \frac{1}{8}\sum_{n=1}^{\ell-1}\|\zeta^{n+1}\|^2_{b^n}\Delta t$$

$$+ \sum_{n=0}^{\ell-1}\frac{n}{16}\{\|\delta\zeta^n\|^2_\phi + |||\delta\zeta^n|||^2_n\}$$

(4.55)

$$\leq K_{63}\{|||\zeta^0|||^2_0 + h^{2r} + h^{2s} + h^{2r+2s-6} + (\Delta t)^2\}$$

$$+ K_{64}\sum_{n=1}^{\ell-1}[n\|\delta\zeta^{n-1}\|^2_{L^\infty} + \Delta t](\|\zeta^n\|^2_{b^{n-1}}\, n\Delta t + \|\zeta^n\|^2_\phi) + \frac{\rho_1'^2\varepsilon_1}{\Delta t}\sum_{n=0}^{\ell-1}|||\delta\zeta^n|||^2_n .$$

Then by letting

(4.56) $\qquad \varepsilon_1 < (32\rho_1'^2)^{-1}$

where ρ_1' is given to satisfy (4.47) and using (3.10), we can hide the last term on the right of (4.55) in the corresponding term on the left side of (4.55).

In order to apply the discrete Gronwall lemma to (4.55), we wish to show that there exists a constant $K_{65} > 0$ such that

(4.57) $\qquad \sum_{n=1}^{\ell-1} n\|\delta\zeta^{n-1}\|^2_{L^\infty} < K_{65}$.

Since for $n \geq 2$, $\frac{n}{n-1} \leq 2$, we have

$$\sum_{n=1}^{\ell-1} n\|\delta\zeta^{n-1}\|^2_{L^\infty} \leq \|\delta\zeta^0\|^2_{L^\infty} + \sum_{n=2}^{\ell-1}\frac{n}{n-1}(n-1)\|\delta\zeta^{n-1}\|^2_{L^\infty}$$

(4.58)

$$\leq \|\delta\zeta^0\|^2_{L^\infty} + 2\sum_{n=1}^{\ell-2} n\|\delta\zeta^n\|^2_{L^\infty} ,$$

and our starting procedure satisfies

(4.59) $\qquad \|\delta\zeta^0\|^2_{L^\infty} \leq K_{67}$

it suffices to show that

(4.60) $\qquad \sum_{n=1}^{\ell-2} n\|\delta\zeta^n\|^2_{L^\infty} \leq K_{68}$.

We shall use an induction argument as in [19, 6, 16] to yield (4.60). For $\ell = 2$, the inequality (4.55) and the estimate (3.20) imply that

$$\|\delta\zeta^1\|_\phi^2 \le K_{69}\{|||\zeta^0|||_0^2 + (\|\delta\zeta^0\|_{L^\infty}^2 + \Delta t)|||\zeta^1|||_0^2$$

(4.61) $$+ h^{2r} + h^{2s} + h^{2r+2s-6} + (\Delta t)^2\}$$

$$\le K_{70}\{h^{2r} + h^{2s} + h^{2r+2s-6} + (\Delta t)^2\}.$$

If $r \ge 2$, $s \ge 2$, and $\Delta t > 0$ satisfy

(4.62)
a) $\Delta t < h^{d/2}$
b) $r+s > \frac{d}{2} + 3$

then for Δt and h sufficiently small,

(4.63) $$\|\delta\zeta^1\|_\phi^2 \le h^d.$$

Assume the following induction hypothesis:

(4.64) $$\sum_{n=1}^{k} n\|\delta\zeta^n\|_\phi^2 \le h^d, \quad \text{for } 1 \le k \le \ell-2.$$

Using the inverse hypothesis (2.2.a) and (4.64) we see that

(4.65) $$\sum_{n=1}^{\ell-2} n\|\delta\zeta^n\|_{L^\infty}^2 \le \frac{K_0^2}{\phi_*} h^{-d} \sum_{n=1}^{\ell-2} n\|\delta\zeta^n\|_\phi^2 \le K_0^2/\phi_*.$$

Then, with $K_{65} = K_{67} + 2K_0^2/\phi_*$, we apply the discrete Gronwall lemma in (4.55), to obtain

$$\|\zeta^\ell\|_\phi^2 + (\|\zeta^\ell\|_\phi^2 + \|\zeta^\ell\|_{b^{\ell-1}}^2)\ell\Delta t + \sum_{n=1}^{\ell-1}\|\zeta^{n+1}\|_{b^n}^2\Delta t + \sum_{n=1}^{\ell-1} n(\|\delta\zeta^n\|_\phi^2 + |||\delta\zeta^n|||_n^2)$$

(4.66)

$$\le K_{71}\{h^{2r} + h^{2s} + h^{2r+2s-6} + (\Delta t)^2\},$$

where

$$K_{71} \le K_{63}\exp\{K_{64}[T + K_{67} + 2K_0^2/\phi_*]\}.$$

We then see that for h and Δt sufficiently small, our induction argument is completed. Since (4.66) holds for each ℓ from $\ell=1$ to $\ell=N$, we have

(4.67) $$\sup_{t^n}\|\zeta^n\| + \sup_{t^n}(\|\zeta^n\|_1^2\, n\Delta t) \le K_{72}\{h^r + h^s + h^{r+s-3} + \Delta t\}.$$

Then for $u \in L^\infty(J;H^r)$, Lemma 2.2 and the triangle inequality yield the desired result. //

The assumptions $c \in L^\infty(J;H^r)$ and $\frac{\partial c}{\partial t} \in L^2(J;H^r)$ made for Theorem 4.2 are not balanced. We shall next obtain the same a-priori error estimates as in Theorem 4.2 under the weakened assumption that $\frac{\partial c}{\partial t} \in L^2(J;H^{r-1})$ using the results of Lemma 2.4. Note that more computing effort is required with the weaker assumption in this case.

<u>Corollary 4.3.</u> Let (c,p) satisfy (1.3) (with $f_1 \equiv 0$ and $b = b(x,c)$) and (C^n,P^n) satisfy (2.40) (as modified by the iterative procedure of Section 3). Assume (3.20) holds and Ω is H^3-regular. If we obtain a norm reduction of the form (3.18) with

(4.68)
a) $\rho_1' \le h$
b) $\rho_2 \le \frac{1}{4}(a_*/a^*)^{1/2}$

then there exist positive constants K_{72}, h_0, and τ_0 such that if $\Delta t \le \tau_0$ and $h \le h_0$,

(4.69) $$\sup_{t^n}\|C-c\| \le K_{72}\{h^r + h^s + h^{r+s-3} + \Delta t\}.$$

<u>Proof</u>: Recall from (4.7) that (4.22) holds under the assumption that $\frac{\partial c}{\partial t} \in L^2(J;H^{r-1})$. We must now replace the bound on the first term on the left of (4.24). As in (4.24),

$$n\Delta t\left|\left(\phi\left(\frac{\partial c^{n+1}}{\partial t} - d_t\tilde{c}^n\right),\delta\zeta^n\right)\right| \le K_{73}\Delta t\left\{\left\|\frac{\partial\zeta^n}{\partial t}\right\|^2 + (\Delta t)^2\right\} + \frac{n}{16}\|\delta\zeta^n\|_\phi^2$$

(4.70)

$$\le K_{73}\,\Delta t\{K_4^2 h^{2(r-1)}\left[\|c^n\|_{r-1} + \left\|\frac{\partial c^n}{\partial t}\right\|_{r-1}\right]^2 + (\Delta t)^2\} + \frac{n}{16}\|\delta\zeta^n\|_\phi^2.$$

Similarly the weaker assumption on $\frac{\partial c}{\partial t}$ will yield a weaker bound in (4.29). We note that these bounds enter the rest of the analysis through the last term on the right of (4.22). If $\rho_1'^2$ were independent of h, the final estimate (4.69) would have h^r replaced by h^{r-1}. In order to regain the lost power of h, we must iterate sufficiently often that

(4.71) $$\rho_1' \le K h.$$

The rest of the proof follows as before. //

As was pointed out earlier, a case of great physical interest is when $b = b(x)$ from (1.1) has only spatial dependence. Then the matrices to be inverted at each time step do not change with time. In this case, once $L^n \equiv L^0$ has been factored and stored, the solution of (3.2.a) at each time step only requires the formation of a new right hand side and a simple backsolve using the factored L^0. We then clearly get results corresponding to Theorem 4.2 with the iteration of (2.40.a) replaced by a simple backsolve.

Theorem 4.4. Let (c,p) satisfy (1.3) with $f_1 \equiv 0$ and $b = b(x)$ and (C^n, P^n) satisfy (2.40) (as modified in Section 3). Let (3.20) be satisfied and Ω be H^3-regular. If we obtain a norm reduction of the form (3.18.b) with

$$\rho_2 \le \frac{1}{4}(a_*/a^*)^{1/2},$$

then there exist positive constants K_{74}, h_0, and τ_0 such that, if $\Delta t \le \tau_0$ and $h \le h_0$,

(4.72) $$\sup_{t^n} \|C - c\| \le K_{74}(h^r + h^s + h^{r+s-3} + \Delta t).$$

Proof: The result follows directly from the proof of Theorem 4.1. //

Clearly, the use of (2.40) and its modifications will only yield $O(\Delta t)$ time-discretization errors while use of (2.41) and (2.40.b) can yield $O((\Delta t)^2)$ errors. The Crank-Nicolson time-stepping method does not have the dissipation which is present in the backwards difference method presented in (2.40.a). Without some dissipation, use of the preconditioning method with iterative stabilization such as presented in Section 3 requires a norm reduction of the order Δt at each time step [6]. In [3] Bramble and Sammon are analyzing iterative methods for higher order time-stepping procedures which have better dissipation properties. It is also noted in [6] that if the preconditioner is updated after each $(N)^{1/2}$ time steps, then a norm reduction of $O((\Delta t)^{1/2})$ is produced with each iteration and two iterations will yield the required $O(\Delta t)$ norm reduction.

Using one of the options of iterating $O(\log \frac{1}{\Delta t})$ times per time step or updating and refactoring the preconditioner after each $(N)^{1/2}$ time steps and iterating at most twice per time step will yield results similar to those presented above, for (C,P) determined by the iterative modifications of (2.41) and (2.40.b), which have time-truncation errors of the order $O((\Delta t)^2)$. Slightly more smoothness on p and c must be assumed. We shall not present the particulars here.

We next consider the extensions of the above analysis to single nonlinear parabolic equations with nonlinear boundary conditions. In order to use the iterative procedure most efficiently for the extrapolated Crank-Nicolson Galerkin procedure we shall introduce dissipation into the scheme by making the assumptions

(4.73) $$\Delta t \le K^* h^2.$$

This is really no restriction if piecewise cubics or higher order elements are used for M_h. Without this restriction, more iterations or refactoring, as described above, will be required. Note that under (2.2) and (4.73), we have

(4.74) $$\Delta t\|\zeta^n\|_1^2 \le \frac{\Delta t K_0^2}{h^2}\|\zeta^n\|^2 \le K_0^2 K^*\|\zeta^n\|^2.$$

Since the Crank-Nicolson-Galerkin method yields $O((\Delta t)^2)$ time-discretization errors, instead of using linear extrapolation to start the iterative procedure as in (3.5), we shall use quadratic extrapolation. We thus assume that our iterative procedure yields a norm reduction of the form

(4.75) $$|||C^{n+1} - \bar{C}^{n+1}|||_n \le \rho_1' |||\delta^3 C^n|||_n^2, \quad n \ge 2,$$

where

(4.76)

a) $$|||\cdot|||_n = \|\cdot\|_\phi + \frac{(\Delta t)^{1/2}}{2}\|\cdot\|_{b^n}$$

b) $$\delta^3 C^n = C^{n+1} - 3C^n + 3C^{n-1} - C^{n-2}.$$

Corresponding norm reductions will be assumed for $n = 1$ and $n = 0$ (see [6]). See [6, 16] for variations of (Q) and (R) for this parabolic problem. We then obtain the following theorem.

Theorem 4.5. Let c satisfy (1.4) (with $f_1^* \equiv 0$) and C satisfy (2.42) (with iterative modifications). Assume (3.20) and (4.73) are satisfied and that $\frac{\partial c}{\partial t} \in L^2(J;H^r)$. If we obtain a norm reduction of the form (4.75) with

$$\rho_1' \le \left\{8\left(1 + \frac{b^* K_0 K^*}{b_*}\right)\right\}^{-1} , \tag{4.77}$$

then there exists positive constants K_{75}, τ_0, and h_0, such that if $\Delta t \le \tau_0$ and $h \le h_0$,

$$\sup_{t^n} \|C-c\| \le K_{75} \{h^r + (\Delta t)^2\} . \tag{4.78}$$

Proof: Subtracting (2.12) (modified slightly for this problem) from (2.42), we obtain

$$\begin{aligned}(\phi d_t \zeta^n, \chi) + (b(EC^n)\nabla\zeta^{n+\frac{1}{2}}, \nabla\chi) &= (\phi[\frac{\partial c}{\partial t}^{n+\frac{1}{2}} - d_t \tilde{c}^n], \chi)\\ &+([b(c^{n+\frac{1}{2}}) - b(EC^n)]\nabla\tilde{c}^{n+1}, \nabla\chi) - \lambda(\xi^{n+\frac{1}{2}}, \chi)\\ &+ ([u(c^{n+\frac{1}{2}}) \cdot \nabla\tilde{c}^{n+\frac{1}{2}} - u(EC^n)\cdot\nabla C^n], \chi)\\ &+ (g(\tilde{c}^{n+\frac{1}{2}}) - g(EC^n), \chi)\\ &+ (\phi\frac{C^{n+1} - \overline{C}^{n+1}}{\Delta t}, \chi) + (b(EC^n)\nabla(C^{n+1} - \overline{C}^{n+1}), \nabla\chi), \quad \chi \in M_h .\end{aligned} \tag{4.79}$$

The test function $\chi = \zeta^{n+\frac{1}{2}}$ will correspond with $\chi = \zeta^{n+1}$ in the earlier analysis. We refer the reader to [6, 10, 16] for methods for treating Extrapolated Crank-Nicolson-Galerkin methods and extending the above analysis to the present case. In order to show how we overcome the difficulties encountered with the boundary terms in [5] while using the test function $\chi = \zeta^{n+\frac{1}{2}}$, we shall present explicit bounds for the sixth term on the right of (4.79). We use (4.9) and (4.24) to see that

$$\begin{aligned}&\left|\sum_{n=1}^{\ell-1} (g(\tilde{c}^{n+\frac{1}{2}}) - g(EC^n), \zeta^{n+\frac{1}{2}})\right|\\ &\le K_{76} \sum_{n=1}^{\ell-1} \left| ((\Delta t)^2 + \zeta^{n+\frac{1}{2}} - \frac{1}{2}[\delta\zeta^n - \delta\zeta^{n-1}], \zeta^{n+\frac{1}{2}})\right|\\ &\le \frac{1}{16} \sum_{n=1}^{\ell-1} \left\|\zeta^{n+\frac{1}{2}}\right\|_{b^n}^2 + \frac{1}{16(\Delta t)^{1/2}} \sum_{n=0}^{\ell-1} \|\delta\zeta^n\|_\phi^2 + K_{77} \sum_{n=0}^{\ell} \{\|\zeta^n\|_\phi^2 + (\Delta t)^4\}.\end{aligned} \tag{4.80}$$

Then using (4.74) and (4.75) as in (4.14), we obtain

$$\begin{aligned}&\left|(\phi\frac{C^{n+1} - \overline{C}^{n+1}}{\Delta t}, \zeta^{n+\frac{1}{2}}) + \frac{1}{2}(b(EC^n)\nabla(C^{n+1} - \overline{C}^{n+1}), \nabla\zeta^{n+\frac{1}{2}})\right|\\ &\le K_{78}\{\|\zeta^{n+1}\|_\phi^2 + \|\zeta^n\|_\phi^2 + (\Delta t)^4\} + \frac{\rho_1'^2 \varepsilon_1}{(\Delta t)^2}\{\|\delta\zeta^n\|_\phi^2 + \|\delta\zeta^{n-1}\|_\phi^2 + \|\delta\zeta^{n-2}\|_\phi^2\}.\end{aligned} \tag{4.81}$$

Then combining these and related estimates, we obtain

$$\begin{aligned}&\frac{1}{2}\{\|\zeta^\ell\|_\phi^2 + \sum_{n=1}^{\ell-1}\left\|\zeta^{n+\frac{1}{2}}\right\|_{b^n}^2 \Delta t\} \le K_{79}\{\sum_{n=0}^{\ell} \|\zeta^n\|_\phi^2 \Delta t + |||\zeta^0|||_0^2\\ &+ h^{2r} + (\Delta t)^4\} + \frac{\rho_1'^2 \varepsilon_1}{\Delta t} \sum_{n=0}^{\ell-1} \|\delta\zeta^n\|_\phi^2 .\end{aligned} \tag{4.82}$$

We note that (4.82) corresponds to (4.22). The rest of the proof follows very closely the proof of Theorem 4.2. The modifications for treating the extrapolated coefficients can be found in [6, 10, 16]. //

We finally note that as in Corollary 4.3, if one iterates $O(h)$ at each time step, a slight modification of Lemma 2.4 will yield (4.78) under the weaker assumption that $\frac{\partial c}{\partial t} \in L^2(J;H^{r-1})$.

5. Computational Considerations

In this section we shall consider some rough operation counts to estimate the computational complexity of the methods presented here. We shall see that the preconditioned conjugate gradient iterative methods presented allow us to obtain near optimal order work estimates. Thus these methods are very efficient computationally.

Recall that we have two space variables $(d = 2)$. George [13] has shown in some special cases that with $M_1 = M_1(h) = \dim M_h$, the procedure of setting up and factoring L^n requires $O(M_1^{3/2})$ operations and that the solution of (3.2.a), given the factorization, requires $O(M_1 \log M_1)$ operations. Similarly, the work involved in setting up and factoring A^n and solving (3.2.b) using this factorization are $O(M_2^{3/2})$ and $O(M_2 \log M_2)$ respectively. Hoffman, Martin and Rose [14] have shown that such bounds are minimal. Thus, if we conjecture the validity of the above estimates for our problem and refactor L^n and A^n and solve (3.2) at each time step, the total amount of work done is

$$O(N(M_1^{3/2} + M_1 \log M_1) + M_2^{3/2} + M_2 \log M_2)) = O(N(M_1^{3/2} + M_2^{3/2})) , \tag{5.1}$$

where N is the total number of time steps $(N \approx \frac{1}{\Delta t})$. We note that the work of refactorization dominates the estimates.

Using the preconditioned iterative methods presented here, one does not need to refactor at every time step. Instead only one factorization of L^0 and A^0 need be done. Then let κ_1 and κ_2 be the number of iterations needed to achieve the necessary norm reductions in (3.18)(a) and (b) respectively. We note that κ_2 is always a constant, independent of h, n and Δt. For Theorem 1, when $b = b(x,c,\nabla p)$, we must have $\kappa_1 = O(\log \frac{1}{\Delta t}) = O(\log N)$ to achieve a norm reduction of $O(\Delta t)$. Thus the total work for Theorem 4.1 is

$$\begin{aligned} &O(M_1^{3/2} + N \log N\, M_1 \log M_1 + M_2^{3/2} + N\, \kappa_2 M_2 \log M_2) \\ &= O(N\, M_1 \log N \log M_1 + N\, M_2 \log M_2) \end{aligned} \tag{5.2}$$

since for $r \geq 2$, $N \approx \frac{1}{\Delta t} \approx \frac{1}{h^r} = O(M_1^{r/2}) \geq M_1$. For Theorem 4.2, when $b = b(x,c)$, κ_1 can be chosen as a constant, independent of h, n, and Δt. Thus the total work for Theorem 4.2 is

$$\begin{aligned} &O(M_1^{3/2} + N\, \kappa_1 M_1 \log M_1 + M_2^{3/2} + N\, \kappa_2 M_2 \log M_2) \\ &= O(N\, M_1 \log M_1 + N\, M_2 \log M_2) . \end{aligned} \tag{5.3}$$

For Corollary 4.3, we must choose $\kappa_1 = O(\log \frac{1}{h}) = O(\log M_1^{1/2}) = O(\log M_1)$ in order to reduce the smoothness assumptions, and the resulting total work is

$$\begin{aligned} &O(M_1^{3/2} + N \log M_1\, M_1 \log M_1 + M_2^{3/2} + N\, \kappa_2 M_2 \log M_2) \\ &= O(N\, M_1 (\log M_1)^2 + N\, M_2 \log M_2) . \end{aligned} \tag{5.4}$$

Since the total number of unknowns in these problems are

$$O(N\, (M_1 + M_2)) , \tag{5.5}$$

we see that (5.2)-(5.4) represent almost optimal order work estimates. A similar result holds for the case of Theorem 4.5.

It is computationally wasteful to iterate exactly κ_1 times at each time step (respectively κ_2 times) in order to achieve the pessimistic bounds given in the statements of the theorems. Instead, one can monitor the norm reduction actually produced at each step of the iteration and stop iterating when sufficient norm reduction is achieved. Additional stopping criteria can be imposed in this monitoring process. See [6] for a discussion stopping criteria for related problems.

In the physical problem (1.1)-(1.2), the pressure p is much smoother in time than a concentration c. In order to take advantage of this difference in smoothness, one can use different time steps for the different systems of equations arising from the pressure and concentration variables. Analysis of this idea for homogeneous boundary conditions appears in [11]. The techniques used above can extend this result to nonlinear boundary conditions. Then the system of linear equations arising from (3.2.b) must be solved only at every $k^{\underline{th}}$ time step where k is determined by the relative smoothnesses of the unknowns. This would clearly be a great computational savings. See [11] for particulars.

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Efficient procedures for time-stepping Galerkin methods for approximating the solution of a coupled nonlinear system for $c=c(x,t)$ and $p=p(x,t)$ with nonlinear Neumann boundary conditions of the form

$$
(*)\quad
\begin{aligned}
&\nabla\cdot[a(x,c)\{\nabla p-\gamma(x,c)\nabla d\}] \equiv -\nabla\cdot u = f_1, && x\in\Omega,\ t\in(0,T],\\
&\nabla\cdot[b(x,c,\nabla p)\nabla c]-u(x,c,\nabla p)\cdot\nabla c = \phi(x)\frac{\partial c}{\partial t}+f_2(c), && x\in\Omega,\ t\in(0,T],\\
&u\cdot\nu = g_1(x,t), && x\in\partial\Omega,\ t\in(0,T],\\
&b\frac{\partial c}{\partial\nu} = g(x,t,c), && x\in\partial\Omega,\ t\in(0,T],\\
&c(x,0)=c_0(x), && x\in\Omega,
\end{aligned}
$$

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abstract - continued

where $\Omega \subset \mathbb{R}^2$, are presented and analyzed. Systems like (*) are possible model systems for describing the miscible displacement of one incompressible fluid by another in a porous medium when flow conditions are prescribed on the boundary. The procedures involve the use of a preconditioned iterative method for approximately solving the different linear systems of equations arising at each time step in a discrete-time Galerkin method. Improvements in starting procedures over many methods are obtained. Some negative-index norm results are obtained which allow weaker smoothness assumptions on $\frac{\partial c}{\partial t}$ than in some previous treatments. Optimal order convergence rates are obtained in most cases for the methods which are computationally more efficient than standard methods. Work estimates of almost optimal order are obtained. The techniques developed are also applied to single nonlinear parabolic equations with nonlinear boundary conditions.