COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING 47 (1984) 73–92
NORTH-HOLLAND

CHAPTER 3

CONVERGENCE ANALYSIS OF AN APPROXIMATION OF MISCIBLE DISPLACEMENT IN POROUS MEDIA BY MIXED FINITE ELEMENTS AND A MODIFIED METHOD OF CHARACTERISTICS

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Received 1 March 1984

A nonlinear system of two coupled partial differential equations models miscible displacement of one incompressible fluid by another in a porous medium. Conservation of mass for the mixture leads to an elliptic equation for pressure, and conservation for the displacing fluid yields a convection-dominated parabolic equation for the concentration of that fluid. A sequential implicit time-stepping procedure is defined, in which the pressure and Darcy velocity of the mixture are approximated simultaneously by a mixed finite element method and the concentration is approximated by a combination of a Galerkin finite element method and the method of characteristics. Optimal-order convergence in L^2 is proved. Time-truncation errors of standard procedures are reduced by time stepping along the characteristics of the hyperbolic part of the concentration equation; temporal and spatial errors are lessened by direct computation of the velocity in the mixed method, as opposed to differentiation of the pressure. Several extensions of these results are outlined.

0. Introduction

Miscible displacement of one incompressible fluid by another in a porous medium Ω over time interval $J = [0, T]$ is modeled by the system

$$-\nabla \cdot \left(\frac{k}{\mu(c)}(\nabla p - \gamma(c)\nabla d)\right) \equiv \nabla \cdot u = q\,, \quad x \in \Omega,\ t \in J, \tag{0.1a}$$

$$\phi\,\frac{\partial c}{\partial t} - \nabla \cdot (D(u)\nabla c - uc) = \tilde{c}q\,, \qquad x \in \Omega,\ t \in J, \tag{0.1b}$$

$$u \cdot n = (D(u)\nabla c - uc) \cdot n = 0\,, \qquad x \in \partial\Omega,\ t \in J, \tag{0.1c}$$

$$c(x, 0) = c_0(x)\,, \qquad x \in \Omega\,. \tag{0.1d}$$

We assume that the medium is vertically homogeneous and take $\Omega \subset \mathbb{R}^2$, except at the end of the paper where extensions to $\Omega \subset \mathbb{R}^3$ are considered. The dependent variables are $p(x, t)$, the pressure in the fluid mixture, and $c(x, t)$, the concentration of a solvent injected into resident oil. In this tertiary oil-recovery process, solvent is injected at certain wells in a petroleum reservoir, mixes with oil to form a single phase, and flows to other wells where oil is produced. (0.1a) and (0.1b) represent conservation of mass for the fluid mixture and the injected solvent, respectively. The coefficients and data in (0.1) are $k(x)$, the permeability of the porous rock; $\mu(c)$, the viscosity of the fluid mixture; $\gamma(x, c)$ and $d(x)$, the gravity coefficient and vertical coordinate; $u(x, t)$, the Darcy velocity of the mixture (volume flowing across a unit cross-section per unit time); $q(x, t)$, representing flow rates at wells, commonly a linear combination of Dirac measures; $\phi(x)$, the porosity (proportion of volume available to porous flow) of the rock; $D(x, u)$, the coefficient of molecular diffusion and (anisotropic velocity-dependent) mechanical dispersion of one fluid into the other; $\tilde{c}(x, t)$, the injected concentration at injection wells and the resident concentration at production wells; and $c_0(x)$, the initial concentration. The initial pressure is determined only up to an additive constant by (0.1a) and (0.1c); this indeterminacy holds at all later times as well, but it is of no consequence since u is uniquely determined by (0.1a), and only u (not p) appears in (0.1b). Related to the indeterminacy is the compatibility condition $\int_\Omega q(x, t)\,\mathrm{d}x = 0$ that must be imposed on the data. A detailed derivation of (0.1) appears in [18].

The principal variable of physical interest in (0.1) is the concentration, $0 \leq c(x, t) \leq 1$, because it shows how much of the reservoir is swept by solvent, or equivalently, how much oil is recovered. In realistic displacements D is quite small, so that (0.1b) for c is strongly convection-dominated. Standard upwind finite difference methods used in the petroleum industry for such problems artificially smear concentration fronts with excessive numerical dispersion and produce solutions that depend strongly on the orientation of the difference grid relative to the streamlines of flow. Other standard techniques without upwinding produce unacceptable nonphysical oscillations in the concentration approximations. In this paper we approximate c by a modified method of characteristics that reduces these difficulties substantially.

This procedure was introduced and analyzed for a single parabolic equation by Douglas and one of the authors in [10], using either finite differences or finite elements to discretize in space. The nine-point finite difference version of the method has been analyzed for (0.1b) in combination with either a five-point difference scheme [6] or a mixed finite element method [5] for (0.1a). The finite element version for (0.1b) has been analyzed with a standard Galerkin procedure for (0.1a) [17]. Optimal-order rates of convergence were obtained in all cases, assuming smooth data. Pironneau [15] has analyzed a closely related finite element procedure for the Navier–Stokes equations from a different viewpoint, allowing D to go to zero while proving suboptimal convergence. In this paper, we analyze the finite element method of [10] applied to (0.1b) with a mixed method for (0.1a); this combination has produced the best numerical results we have seen [13].

The numerical behavior of the modified method of characteristics for (0.1b) depends strongly on the accuracy of the approximation of the velocity u. Thus, it is not surprising that a mixed method, which computes p and u simultaneously without differentiation of p and multiplication by the rough coefficient k/μ, improves the approximation of c. The mixed method considered here was introduced and analyzed for second-order elliptic problems by Raviart and Thomas [16]. For (0.1a), the method has been analyzed in combination with a standard Galerkin procedure for (0.1b) in [8] and [9], using continuous and discrete time, respectively. Optimal results were proved for smooth data; for singular data (e.g., Dirac measures) and μ independent of c, suboptimal convergence was demonstrated in [8]. As noted above, the mixed method has also been analyzed with the nine-point finite difference version of the modified method of characteristics for (0.1b) [5]. A more detailed summary of previous analysis and numerical work with these methods is given in [18].

This paper is organized as follows. In Section 1 we refine the statement of our problem and list the assumptions needed for the convergence analysis. We define the finite element version of the modified method of characteristics in Section 2, using spaces satisfying certain approximation and quasi-regularity properties; we also define a useful projection of c into these spaces. Section 3 defines the mixed method and associated spaces and projections, concluding with the time-stepping algorithm that combines the two methods. Optimal-order convergence is proved in Section 4, and some extensions of the theory are outlined. The proof combines the techniques of [8] and [17], with considerable modification and reorganization.

1. Statement of the problem

We introduce here a nondivergence form of (0.1) that is used in our numerical scheme. We also define certain Sobolev spaces of functions, list the smoothness assumptions on the solution of (0.1), and indicate the properties required of the coefficients.

The nondivergence form is obtained by expanding the convection $(\nabla \cdot (uc))$ term in (0.1b) with the product rule and using (0.1a). This leads to

$$\nabla \cdot u = q, \qquad x \in \Omega,\ t \in J, \tag{1.1a}$$

$$\phi \frac{\partial c}{\partial t} + u \cdot \nabla c - \nabla \cdot (D(u)\nabla c) = (\tilde{c} - c)\tilde{q}, \qquad x \in \Omega,\ t \in J, \tag{1.1b}$$

$$u \cdot n = (D(u)\nabla c) \cdot n = 0, \qquad x \in \partial\Omega,\ t \in J, \tag{1.1c}$$

$$c(x, 0) = c_0(x), \qquad x \in \Omega, \tag{1.1d}$$

where $\tilde{q} = \max\{q, 0\}$ is nonzero at injection wells only. To avoid technical boundary difficulties associated with the modified method of characteristics for (1.1b), we assume that Ω is a rectangle and that (1.1) is Ω-periodic. This is physically reasonable, because the no-flow condition (1.1c) can be treated as a reflection boundary, and because boundary effects in reservoir simulation are of considerably less interest than interior flow patterns. Throughout the rest of this paper, all functions will be assumed to be spatially Ω-periodic. The boundary conditions (1.1c) can be dropped.

On Ω, we define the following Sobolev spaces and norms:

$$L^2(\Omega)=\left\{f:\int_\Omega |f|^2\,\mathrm{d}x<\infty\right\}, \qquad \|f\|=\left[\int_\Omega |f|^2\,\mathrm{d}x\right]^{1/2},$$

$$L^\infty(\Omega)=\{f:\operatorname*{ess\,sup}_\Omega |f|<\infty\}, \qquad \|f\|_{L^\infty}=\operatorname*{ess\,sup}_\Omega |f|,$$

$$H^m(\Omega)=\left\{f:\frac{\partial^{|\alpha|}f}{\partial x^\alpha}\in L^2(\Omega)\text{ for }|\alpha|\leq m\right\}, \qquad \|f\|_m=\left[\sum_{|\alpha|\leq m}\left\|\frac{\partial^{|\alpha|}f}{\partial x^\alpha}\right\|^2\right]^{1/2}, \quad m\geq 0,$$

$$W^m_\infty(\Omega)=\left\{f:\frac{\partial^{|\alpha|}f}{\partial x^\alpha}\in L^\infty(\Omega)\text{ for }|\alpha|\leq m\right\}, \qquad \|f\|_{W^m_\infty}=\max_{|\alpha|\leq m}\left\|\frac{\partial^{|\alpha|}f}{\partial x^\alpha}\right\|_{L^\infty}, \quad m\geq 0.$$

In particular, $H^0(\Omega)=L^2(\Omega)$ and $W^0_\infty(\Omega)=L^\infty(\Omega)$. The inner product on $L^2(\Omega)$ is denoted by

$$(f,g)=\int_\Omega fg\,\mathrm{d}x.$$

We also require spaces that incorporate time dependence. Let $[a,b]\subset J$ and let X be any of the spaces just defined. If $f(x,t)$ represents functions on $\Omega\times[a,b]$, we set

$$H^m(a,b;X)=\left\{f:\int_a^b\left\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\right\|_X^2\mathrm{d}t<\infty,\ \alpha\leq m\right\},$$

$$\|f\|_{H^m(a,b;X)}=\left[\sum_{\alpha=0}^m\int_a^b\left\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\right\|_X^2\mathrm{d}t\right]^{1/2}, \quad m\geq 0,$$

$$W^m_\infty(a,b;X)=\left\{f:\operatorname*{ess\,sup}_{[a,b]}\left\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\right\|_X<\infty,\ \alpha\leq m\right\},$$

$$\|f\|_{W^m_\infty(a,b;X)}=\max_{0\leq\alpha\leq m}\ \operatorname*{ess\,sup}_{[a,b]}\left\|\frac{\partial^\alpha f}{\partial t^\alpha}(\cdot,t)\right\|_X, \quad m\geq 0,$$

$$L^2(a,b;X)=H^0(a,b;X), \qquad L^\infty(a,b;X)=W^0_\infty(a,b;X).$$

If $[a,b]=J=[0,T]$, we drop it from the notation. We also drop Ω; thus, we write $L^\infty(W^1_\infty)$ for $L^\infty(0,T;W^1_\infty(\Omega))$.

If $f=(f_1,f_2)$ is a vector function, such as the velocity u in (1.1), we say that $f\in X$ if $f_1\in X$ and $f_2\in X$. We also define the special vector-function spaces and norms

$$H^m(\mathrm{div};\Omega)=\{f:f_1,f_2,\nabla\cdot f\in H^m(\Omega)\},$$

$$\|f\|_{H^m(\mathrm{div})}=[\|f_1\|_m^2+\|f_2\|_m^2+\|\nabla\cdot f\|_m^2]^{1/2}, \quad m\geq 0,$$

$$H(\mathrm{div};\Omega)=H^0(\mathrm{div};\Omega).$$

Our assumptions on the regularity of the solution of (1.1) are denoted collectively by

$$
\text{(R)}\qquad
\begin{aligned}
&c \in L^\infty(H^{l+1}) \cap H^1(H^{l+1}) \cap L^\infty(W^1_\infty) \cap H^2(L^2)\,,\\
&p \in L^\infty(H^{k+1})\,,\\
&u \in L^\infty(H^{k+1}(\mathrm{div})) \cap L^\infty(W^1_\infty) \cap W^1_\infty(L^\infty) \cap H^2(L^2)\,,
\end{aligned}
$$

where $l \geq 1$ and $k \geq 0$ are integers to be chosen for the approximation schemes. In practice, l and k are the degrees of piecewise polynomials approximating c and p, respectively.

Note that p and u are required to have the same order of smoothness. This might seem out of balance, since u depends on ∇p. However, in the physical problem the coefficient k/μ may be quite rough or even discontinuous. If, for example, k is discontinuous at an interface of rock types, then the physical p and u should be continuous, but ∇p should be discontinuous. Under such circumstances an assumption such as $p \in H^1$, $u \in H^1(\mathrm{div})$ is quite plausible and even natural.

The hypotheses in (R) enforce tacit conditions on the coefficients in (1.1). We will make explicit use of

$$
\text{(C)}\qquad
\begin{aligned}
&0 < a_* \leq \frac{k(x)}{\mu(c)} \leq a^*\,, \qquad 0 < \phi_* \leq \phi(x) \leq \phi^*\,, \qquad 0 < D_* \leq D(x,u)\,,\\
&\left|\frac{\partial(k/\mu)}{\partial c}(x,c)\right| + \left|\frac{\partial \gamma}{\partial c}(x,c)\right| + |\nabla\phi(x)| + \left|\frac{\partial D}{\partial u}(x,u)\right| + |\tilde q(x,t)| + \left|\frac{\partial \tilde q}{\partial t}(x,t)\right| \leq K^*\,,
\end{aligned}
$$

for constants a_*, a^*, ϕ_*, ϕ^*, D_*, K^*. The assumptions on k/μ, ϕ, and D are reasonable; D is a tensor that depends on the first power of the magnitude of u [18]. However, the bound on $\tilde q$ in the physical problem will be very large, since the reservoir length scale is 3 to 4 orders of magnitude above that of a well diameter. Our analysis will show that our methods are mathematically justified, but it will apply in a practical sense only to a smoothed idealization of (1.1). For realistic convergence rates, it will be necessary to examine the behavior of the approximations as $\tilde q$ tends toward a singular Dirac measure. Of the studies of this physical problem, only [14] has moved in that direction.

2. A modified method of characteristics for the concentration

The modified method of characteristics is a time-stepping procedure that can be combined with any spatial discretization. We define the procedure here and apply it to (1.1b), assuming that a velocity from (1.1a) is known. Then we introduce a finite element mesh, consider a projection of c into the mesh, and show how the spatial and temporal discretizations are combined.

The basic idea is to think of the hyperbolic part of (1.1b), namely, $\phi\, \partial c/\partial t + u \cdot \nabla c$, as a directional derivative. Accordingly, let s denote the unit vector in the direction of (u_1, u_2, ϕ) in $\Omega \times J$, and set

$$\psi(x) = [|u(x)|^2 + \phi(x)^2]^{1/2} = [u_1(x)^2 + u_2(x)^2 + \phi(x)^2]^{1/2}\,.$$

Then (1.1b) can be rewritten in the form

$$\psi \frac{\partial c}{\partial s} - \nabla \cdot (D\nabla c) + \bar{q}c = \bar{q}\tilde{c}. \tag{2.1}$$

Note that (2.1) has the form of the heat equation, so that its numerical approximations should be better behaved than those of (1.1b) if a reasonable treatment of the 'time' derivative $\partial c/\partial s$ can be found.

Partition J into $0 = t^0 < t^1 < \cdots < t^N = T$, with $\Delta t_c^n = t^n - t^{n-1}$. Our analysis is valid for variable time steps, but we drop the superscript from Δt_c for convenience. For functions f on $\Omega \times J$, we write $f^n(x)$ for $f(x, t^n)$. Approximate $(\partial c^n/\partial s)(x) = (\partial c/\partial s)(x, t^n)$ by a backward difference quotient in the s-direction,

$$\frac{\partial c^n}{\partial s}(x) \simeq \frac{c^n(x) - c^{n-1}\left(x - \dfrac{u(x)}{\phi(x)}\Delta t_c\right)}{\Delta t_c \sqrt{1 + |u(x)|^2/\phi(x)^2}} \tag{2.2}$$

If we let $\bar{x} = x - (u(x)/\phi(x))\Delta t_c$ and $\bar{f}(x) = f(\bar{x})$, then

$$\psi \frac{\partial c^n}{\partial s} \simeq \phi \frac{c^n - \bar{c}^{n-1}}{\Delta t_c}. \tag{2.3}$$

Since the problem is Ω-periodic, $\bar{c}^{n-1}$ is always defined; the tangent to the characteristic (i.e., the s-segment) cannot cross a boundary to an undefined location. The difference quotient relates the concentration at a given x at time t^n to the concentration that would flow to x from time t^{n-1} if the problem were purely hyperbolic.

The time difference (2.3) will be combined with a standard Galerkin procedure in the space variables. For $h_c > 0$ and an integer $l \geq 1$, let $M \subset W_\infty^1(\Omega)$ be a family of finite-dimensional subspaces indexed by h_c and having the following approximation and inverse properties:

$$(\mathrm{A_c}) \quad \begin{aligned} &\inf_{\chi \in M} [\|f-\chi\| + h_c\|f-\chi\|_1 + h_c(\|f-\chi\|_{L^\infty} + h_c\|f-\chi\|_{W_\infty^1})] \leq K_0 h_c^m \|f\|_m, \\ &2 \leq m \leq l+1, \end{aligned}$$

$$(\mathrm{I_c}) \quad \begin{aligned} &\|\chi\|_{W_\infty^1} \leq K_0 h_c^{-1}\|\chi\|_1, \qquad \|\chi\|_{L^\infty} \leq K_0 h_c^{-1}\|\chi\|, \qquad \|\chi\|_1 \leq K_0 h_c^{-1}\|\chi\| \\ &\text{for all } \chi \in M, \end{aligned}$$

where K_0 is independent of h_c. These properties hold, for example, for continuous piecewise polynomials of degree $\leq l$ on a quasi-uniform mesh of diameter $\leq h_c$.

Our convergence analysis will use a technique of one of the authors [19] that relies on a projection of the exact concentration c into M. If u is the exact Darcy velocity, define $\tilde{C}(\cdot, t) \in M$ by

$$\begin{aligned} &(D(u(t))\nabla\tilde{C}(t), \nabla\chi) + (\tilde{C}(t), \chi) + (\bar{q}(t)\tilde{C}(t), \chi) = \\ &\quad = (D(u(t))\nabla c(t), \nabla\chi) + (c(t), \chi) + (\bar{q}(t)c(t), \chi) \\ &\quad = -\left(\phi \frac{\partial c}{\partial t}(t), \chi\right) - (u(t)\cdot\nabla c(t), \chi) + (c(t), \chi) + (\bar{q}(t)\tilde{c}(t), \chi), \quad \chi \in M, t \in J. \end{aligned} \tag{2.4}$$

As in [11, 17], we can use (R), (C), $(\mathrm{A_c})$, and $(\mathrm{I_c})$ to obtain the following facts about $\tilde{C}$:

$$\|c-\tilde{C}\|_{L^\infty(L^2)}+h_c\|c-\tilde{C}\|_{L^\infty(H^1)}\le K_1h_c^m\|c\|_{L^\infty(H^m)}\,, \tag{2.5}$$

$$\left\|\frac{\partial}{\partial t}(c-\tilde{C})\right\|_{L^2(L^2)}\le K_1h_c^m\|c\|_{H^1(H^m)}\,,\quad 2\le m\le l+1\,, \tag{2.6}$$

$$\|\tilde{C}\|_{L^\infty(W^1_\infty)}\le K_1\,, \tag{2.7}$$

where K_1 is independent of c and h_c and depends on $\|u\|_{W^1_\infty(L^\infty)}$ and D_*. We will define a numerical approximation C of c in (3.10) below; with (2.5) known, the convergence analysis will have only to estimate $\|C-\tilde{C}\|$.

We can obtain a weak form of (2.1) by multiplying by a test function in $H^1(\Omega)$ and integrating by parts in the diffusion-dispersion term. A Galerkin discretization of this weak form using M and the characteristic backward difference in (2.3) is given by $C^0_*, C^1_*, \ldots, C^N_*\in M$ such that

$$\begin{aligned}&C^0_*=\tilde{C}^0\,,\\ &\left(\phi\,\frac{C^n_*-\bar{C}^{n-1}_*}{\Delta t_c},\chi\right)+(D(u^n)\nabla C^n_*,\nabla\chi)+\tilde{q}^nC^n_*,\chi)=(\tilde{q}^n\tilde{c}^n,\chi)\,,\quad \chi\in M,\ n\ge 1\,.\end{aligned} \tag{2.8}$$

In practice, u^n must be replaced by a numerical approximation to be determined in the next section; an analogue of the translate $\bar{x}$ using that approximation will be defined.

Note that all occurrences of C^n_* are standard; the translation along characteristics using $\bar{x}$ applies only to C^{n-1}_*. By thus looking *backward* in time along characteristics, we make it possible to solve (2.8) on a static or simply-defined dynamic mesh. Schemes that look forward along characteristics, such as moving-point or front-tracking methods, are difficult to implement in two or three dimensions; these difficulties do not apply to our method.

Note also that (2.8) leads to a symmetric positive-definite matrix at each time step, unlike standard methods in which the dominant convection term is nonsymmetric. Thus, (2.8) is more suitable than standard methods for solution by sparse iterative algorithms, which are necessary when the number of nodes in the spatial mesh is large.

3. A mixed method for the pressure and velocity

The modified method of characteristics in (2.8) requires an accurate approximation of the velocity u^n in order to translate well along characteristics. This approximation will be provided by the mixed finite element method described in this section. We define a coupled weak form of (0.1a), discretize with special finite element spaces, and introduce projections of the exact pressure and velocity into those spaces. Then we exhibit our fully discrete coupled time-stepping procedure for (1.1).

The weak form of (0.1a) seeks $p\in L^2(\Omega)$ and $u\in H(\mathrm{div};\Omega)$. Since p is only determined up to an additive constant, all references to test functions in L^2, L^2 norms of p and of its approximations, and so on, should be understood to mean the quotient space $L^2/\{$constant functions$\}$. Separate (0.1a) into two equations,

$$u = -\frac{k}{\mu(c)}(\nabla p - \gamma(c)\nabla d), \quad x \in \Omega,\ t \in J, \tag{3.1}$$

$$\nabla \cdot u = q, \qquad x \in \Omega,\ t \in J, \tag{3.2}$$

representing Darcy's law and conservation of mass, respectively. For $\kappa \in L^\infty(\Omega)$, α, $\beta \in H(\mathrm{div}; \Omega)$, and $\pi \in L^2(\Omega)$, define the bilinear forms

$$A(\kappa; \alpha, \beta) = \left(\frac{\mu(\kappa)}{k}\alpha, \beta\right), \tag{3.3a}$$

$$B(\alpha, \pi) = -(\nabla \cdot \alpha, \pi); \tag{3.3b}$$

in (3.3a), the inner product is for vector functions in $L^2(\Omega)$. Multiply (3.1) by μ/k and a test function $v \in H(\mathrm{div}; \Omega)$, integrate over Ω, and integrate $(\nabla p, v)$ by parts. Multiply (3.2) by a test function $w \in L^2(\Omega)$ and integrate over Ω. Then (3.1)–(3.2) is equivalent to the time-parametrized saddle-point problem of finding a map $(u, p): J \to H(\mathrm{div}; \Omega) \times L^2(\Omega)$ such that

$$A(c; u, v) + B(v, p) = (\gamma(c)\nabla d, v), \quad v \in H(\mathrm{div}; \Omega), \tag{3.4a}$$

$$B(u, w) = -(q, w), \qquad w \in L^2(\Omega). \tag{3.4b}$$

For $h_p > 0$, we discretize (3.4) in space on a quasi-uniform triangularization or quadrilateralization of Ω with elements of diameter $\leqslant h_p$. Let $V^k \subset H(\mathrm{div}; \Omega)$ and $W^k \subset L^2(\Omega)$ be Raviart–Thomas [16] spaces of index $k \geqslant 0$ for this mesh. For example, if the mesh were rectangular, the first component of V^k would be continuous piecewise polynomials of degree $\leqslant k+1$ in the x_1-direction tensored with discontinuous ones of degree $\leqslant k$ in the x_2-direction, the second component would be the reverse (thus $\nabla \cdot V^k \subset L^2$), and W^k would be the tensor product of discontinuous polynomials of degree $\leqslant k$ in both directions. These spaces possess the approximation and inverse properties

$$\inf_{v \in V^k} \|f - v\| \leqslant K_2 \|f\|_m h_p^m,$$

$$(\mathrm{A_p}) \qquad \inf_{v \in V^k} \|f - v\|_{H(\mathrm{div})} \leqslant K_2 \|f\|_{H^m(\mathrm{div})} h_p^m,$$

$$\inf_{w \in W^k} \|g - w\| \leqslant K_2 \|g\|_m h_p^m, \quad 1 \leqslant m \leqslant k+1,$$

$$(\mathrm{I_p}) \qquad \begin{aligned} &\|v\|_{L^\infty} \leqslant K_2 h_p^{-1} \|v\|, \quad v \in V^k, \\ &\|v\|_{W^1_\infty(\mathcal{T})} \leqslant K_2 h_p^{-1} \|v\|_{L^\infty(\mathcal{T})}, \quad v \in V^k,\ \mathcal{T} \text{ an element of the mesh}. \end{aligned}$$

As in (2.4), it is useful to define projections of the exact solutions into the mesh. Define the map $(\tilde{U}, \tilde{P}): J \to V^k \times W^k$ by

$$A(c(t); \tilde{U}(t), v) + B(v, \tilde{P}(t)) = (\gamma(c(t))\nabla d, v)\,, \quad v \in V^k\,, \tag{3.5a}$$

$$B(\tilde{U}(t), w) = -(q(t), w)\,, \tag{3.5b}$$

where $c(t)$ is the exact solution of (1.1). By arguments in [4, 8], the map exists and $(\mathrm{A_p})$ implies that

$$\begin{aligned}\|u - \tilde{U}\|_{L^\infty(H(\mathrm{div}))} + \|p - \tilde{P}\|_{L^\infty(L^2)} &\leq K_3[\inf_{v \in V^k} \|u - v\|_{H(\mathrm{div})} + \inf_{w \in W^k} \|p - w\|] \\ &\leq K_3(\|u\|_{L^\infty(H^{k+1}(\mathrm{div}))} + \|p\|_{L^\infty(H^{k+1})}) h_{\mathrm{p}}^{k+1}\,. \end{aligned}\tag{3.6}$$

The constant K_3 depends on constants in (C) but is independent of h_{p}, u, p and c. In the same way that (2.7) held, the estimate (3.6) and $(\mathrm{I_p})$ imply that

$$\|\tilde{U}\|_{L^\infty(L^\infty)} \leq K_3\,. \tag{3.7}$$

The mixed method for pressure and velocity, given a concentration approximation C at a time $t \in J$, consists of $U \in V^k$ and $P \in W^k$ such that

$$A(C; U, v) + B(v, P) = (\gamma(c)\nabla d, v)\,, \quad v \in V^k\,, \tag{3.8a}$$

$$B(U, w) = -(q, w)\,, \qquad w \in W^k\,. \tag{3.8b}$$

Existence and uniqueness of U and P is proved in [8], based on ideas of [4, 16]. As in [8], comparison of (3.5) and (3.8) implies that

$$\|U - \tilde{U}\|_{H(\mathrm{div})} + \|P - \tilde{P}\| \leq K_4(1 + \|\tilde{U}\|_{L^\infty})\|c - C\|\,. \tag{3.9}$$

The estimates (3.6) and (3.9) will handle the coupling of concentration and velocity errors in the convergence analysis.

We now present our sequential time-stepping procedure that combines (2.8) and (3.8). In practice, the velocity may change less rapidly in time than the concentration, even if characteristics are taken into account. Thus, it is appropriate to consider using a longer time step for (3.8) than for (2.8). Partition J into pressure time steps $0 = t_0 < t_1 < \cdots < t_M = T$, with $\Delta t_{\mathrm{p}}^m = t_m - t_{m-1}$. Each pressure step is also a concentration step, i.e., for each m there exists n such that $t_m = t^n$; in general, $\Delta t_{\mathrm{p}} > \Delta t_{\mathrm{c}}$. We may vary Δt_{p}, but except for Δt_{p}^1 we drop the superscript. For functions f on $\Omega \times J$, we write $f_m(x)$ for $f(x, t_m)$; thus, subscripts refer to pressure steps and superscripts to concentration steps.

If concentration step t^n relates to pressure steps by $t_{m-1} < t^n \leq t_m$, we require a velocity approximation for (2.8) based on U_{m-1} and earlier values. If $m \geq 2$, take the linear extrapolation of U_{m-1} and U_{m-2} defined by

$$EU^n = \left(1 + \frac{t^n - t_{m-1}}{t_{m-1} - t_{m-2}}\right) U_{m-1} - \frac{t^n - t_{m-1}}{t_{m-1} - t_{m-2}}\, U_{m-2}\,;$$

if $m = 1$, set

$$EU^n = U_0 .$$

We retain the superscript on Δt_p^1 because EU^n is first-order correct in time during the first pressure step and second-order during later steps.

The combined time-stepping procedure is a map $C:\{t^0, t^1, \ldots, t^N\} \to M$ and a map $(U, P):\{t_0, t_1, \ldots, t_M\} \to V^k \times W^k$ defined by

$$C^0 = \tilde{C}^0 , \tag{3.10a}$$

$$\left(\phi \frac{C^n - \hat{C}^{n-1}}{\Delta t_c}, \chi\right) + (D(EU^n)\nabla C^n, \nabla\chi) + (\bar{q}^n C^n, \chi) = (\bar{q}^n \bar{c}^n, \chi), \quad \chi \in M, \quad n \geqslant 1 , \tag{3.10b}$$

$$A(C_m; U_m, v) + B(v, P_m) = (\gamma(C_m)\nabla d, v), \quad v \in V^k , \tag{3.10c}$$

$$B(U_m, w) = -(q_m, w), \qquad w \in W^k, \; m \geqslant 0 , \tag{3.10d}$$

where

$$\hat{C}^{n-1}(x) = C^{n-1}(\hat{x}) = C^{n-1}\left(x - \frac{EU^n(x)}{\phi(x)} \Delta t_c\right).$$

We solve for C^0, then (U_0, P_0), then $C^1, C^2, \ldots, C^{n_1}$ such that $t^{n_1} = t_1$, then (U_1, P_1), and so on.

The convergence analysis will make use of an analogue of $\hat{x}$ defined for the exact velocity u^n. If f is a function on Ω, set

$$\check{f}(x) = f(\check{x}) = f\left(x - \frac{EU^n(x)}{\phi(x)} \Delta t_c\right);$$

the time step t^n will be clear from the context. Throughout the analysis, K will denote a generic constant, independent of h_c, h_p, Δt_c and Δt_p, but possibly depending on constants in (C), norms in (R), and K_i, $0 \leqslant i \leqslant 4$. Similarly, ε will denote a generic small positive constant.

4. A priori error estimates

In this section we demonstrate that the mixed/modified-characteristic approximation (3.10) converges at an optimal rate in $L^2(\Omega)$ to the exact concentration for any order of approximating polynomials ($k \geqslant 0$, $l \geqslant 1$). Optimal error estimates for velocity in $H(\mathrm{div}; \Omega)$ and pressure in $L^2(\Omega)$ follow at once from (3.6) and (3.9). Possible extensions of the analysis to estimates in $H^1(\Omega)$ and to modifications of (3.10) will be noted.

THEOREM 4.1. Suppose that the assumptions (R), (C), (A_c), (I_c), (A_p) *and* (I_p) *hold. For* $l \geqslant 1$ *and* $k \geqslant 0$, *assume that the discretization parameters obey the relations*

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

Then the error of the approximation (3.10) *of* (1.1) *satisfies*

$$\max_{0\leq n\leq N} \|c^n - C^n\| \leq K[h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p^1)^{3/2} + (\Delta t_p)^2] .$$

The size of the Δt_c *term depends principally on* $\|\partial^2 c/\partial\tau^2\|$, *where* τ *approximates the characteristic direction* s *of* (2.1). *The sizes of the* Δt_p *terms depend principally on* $\|\partial u/\partial t\|$ *and* $\|\partial^2 u/\partial t^2\|$. *The spatial terms depend principally on the* H^{l+1} *and* H^{k+1} *norms in* (R).

PROOF. Set $\xi = c - \tilde{C}$, $\zeta = C - \tilde{C}$. By (R) and (2.5) it suffices to show that

$$\sup_n \|\zeta^n\| \leq K[h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p^1)^{3/2} + (\Delta t_p)^2] . \tag{4.1}$$

To obtain a suitable variational equation for ζ, subtract (2.4) from (3.10b) and manipulate to the form

$$\begin{aligned}
&\left(\phi \frac{\zeta^n - \zeta^{n-1}}{\Delta t_c}, \chi\right) + (D(EU^n)\nabla\zeta^n, \nabla\chi) = \\
&\quad = \left(\left[\phi \frac{\partial c^n}{\partial t} + Eu^n \cdot \nabla c^n\right] - \phi \frac{c^n - \check{c}^{n-1}}{\Delta t_c}, \chi\right) + ([u^n - Eu^n]\cdot\nabla c^n, \chi) \\
&\qquad + ([D(u^n) - D(EU^n)]\nabla\tilde{C}^n, \nabla\chi) + \left(\phi \frac{\xi^n - \xi^{n-1}}{\Delta t_c}, \chi\right) - (\xi^n, \chi) - (\bar{q}^n\zeta^n, \chi) \\
&\qquad + \left(\phi \frac{\hat{c}^{n-1} - \check{c}^{n-1}}{\Delta t_c}, \chi\right) - \left(\phi \frac{\hat{\xi}^{n-1} - \check{\xi}^{n-1}}{\Delta t_c}, \chi\right) + \left(\phi \frac{\hat{\zeta}^{n-1} - \check{\zeta}^{n-1}}{\Delta t_c}, \chi\right) \\
&\qquad - \left(\phi \frac{\check{\xi}^{n-1} - \xi^{n-1}}{\Delta t_c}, \chi\right) + \left(\phi \frac{\check{\zeta}^{n-1} - \zeta^{n-1}}{\Delta t_c}, \chi\right), \quad \chi \in M,\ n \geq 1 .
\end{aligned} \tag{4.2}$$

For an L^2 estimate of ζ, choose $\chi = \zeta^n$ as a test function and denote the resulting terms on the right-hand side of (4.2) by $T_1, T_2, \ldots, T_{11}$. The inequality $a(a-b) \geq \frac{1}{2}(a^2 - b^2)$ shows that

$$\frac{1}{2\Delta t_c}[(\phi\zeta^n, \zeta^n) - (\phi\zeta^{n-1}, \zeta^{n-1})] + (D(EU^n)\nabla\zeta^n, \nabla\zeta^n) \leq T_1 + T_2 + \cdots + T_{11} . \tag{4.3}$$

We now estimate T_1 through T_{11}, after which the discrete Gronwall lemma will yield (4.1).

For the estimate of T_1, let

$$\sigma(x) = [\phi(x)^2 + |Eu^n(x)|^2]^{1/2} ,$$

so that

$$\phi \frac{\partial c^n}{\partial t} + Eu^n \cdot \nabla c^n = \sigma \frac{\partial c^n}{\partial \tau(x, t)} ,$$

where τ approximates the characteristic unit vector s of (2.1). Let $\bar{\tau} \in [0, 1]$ parametrize the approximate characteristic tangent from $(x, t^n)[\bar{\tau} = 0]$ to $(\check{x}, t^{n-1})[\bar{\tau} = 1]$. In the same way that we derived (2.3), we see that $\phi(c^n - \check{c}^{n-1})/\Delta t_c$ is a backward-difference approximation of $\sigma\, \partial c^n/\partial\tau$ along the tangent. The usual backward-difference error equation, over a τ-segment of length $\sigma\Delta t_c/\phi$, is

$$\frac{\partial c^n}{\partial \tau} - \frac{\phi}{\sigma}\frac{c^n - \check{c}^{n-1}}{\Delta t_c} = \frac{\phi}{\sigma\Delta t_c}\int_{(\check{x}, t^{n-1})}^{(x, t^n)} [|x - \check{x}|^2 + (t - t^{n-1})^2]^{1/2} \frac{\partial^2 c}{\partial \tau^2}\, \mathrm{d}\tau\,. \tag{4.4}$$

Multiplying (4.4) by σ and taking the square of the $L^2(\Omega)$ norm, we obtain

$$\begin{aligned}\left\|\sigma\frac{\partial c^n}{\partial\tau} - \phi\frac{c^n - \check{c}^{n-1}}{\Delta t_c}\right\|^2 &\leq \int_\Omega \left[\frac{\phi}{\Delta t_c}\right]^2 \left[\frac{\sigma\Delta t_c}{\phi}\right]^2 \left|\int_{(\check{x}, t^{n-1})}^{(x, t^n)} \frac{\partial^2 c}{\partial\tau^2}\,\mathrm{d}\tau\right|^2 \mathrm{d}x \\ &\leq \Delta t_c \left\|\frac{\sigma^3}{\phi}\right\|_{L^\infty} \int_\Omega \int_{(\check{x}, t^{n-1})}^{(x, t^n)} \left|\frac{\partial^2 c}{\partial\tau^2}\right|^2 \mathrm{d}\tau\, \mathrm{d}x \\ &\leq \Delta t_c \left\|\frac{\sigma^4}{\phi^2}\right\|_{L^\infty} \int_\Omega \int_{t^{n-1}}^{t^n} \left|\frac{\partial^2 c}{\partial\tau^2}(\bar{\tau}\check{x} + (1-\bar{\tau})x, t)\right|^2 \mathrm{d}t\, \mathrm{d}x\,. \end{aligned} \tag{4.5}$$

By a change-of-variable argument to be presented in detail in the estimate of T_{10}, $(\bar{\tau}\check{x} + (1-\bar{\tau})x, t)$ can be replaced by (x, t) in (4.5) at the cost of a multiplicative constant. Thus,

$$|T_1| \leq K\left\|\frac{\partial^2 c}{\partial\tau^2}\right\|^2_{L^2(t^{n-1}, t^n; L^2)} \Delta t_c + K\|\zeta^n\|^2\,. \tag{4.6}$$

In (4.6), note that $\tau(x, t)$ is equal to $\tau(x', t^n)$, where x' is such that the approximate characteristic tangent at (x', t^n) passes through (x, t). The difference between $\tau(x, t)$ and the true characteristic direction could be reduced by a modification of the method, in which $\hat{x}$ would be determined by an approximate characteristic polygon corresponding to a partition of $[t^{n-1}, t^n]$ into sub-timesteps. This has been done in practice [13] near wells, where u varies rapidly in space. In any case, for convection-dominated problems the norm of $\partial^2 c/\partial\tau^2$ appearing in (4.6) is much smaller than the corresponding $\partial^2 c/\partial t^2$ of standard procedures, so that time-truncation error is reduced and larger Δt_c is appropriate.

Next, we routinely see that

$$|T_2| \leq \|u^n - Eu^n\|\|\nabla c^n\|_{L^\infty}\|\zeta^n\| \leq K(\Delta t_p)^3\left\|\frac{\partial^2 u}{\partial t^2}\right\|^2_{L^2(t_{m-2}, t_m; L^2)} + K\|\zeta^n\|^2\,, \tag{4.7}$$

where t_{m-2} and t_{m-1} are the previous pressure time levels that define the extrapolation Eu^n at concentration time level t^n. If $t^n \leq t_1$, so that $Eu^n = u_0$ (extrapolation not possible), then the temporal error term is replaced by $K(\Delta t_p^1)^2\|\partial u/\partial t\|^2_{L^\infty(t_0, t_1; L^2)}$.

For the T_3 bound, note that by (3.6),

$$\|Eu^n - E\tilde{U}^n\| \leq K\|u_{m-1} - \tilde{U}_{m-1}\| + K\|u_{m-2} - \tilde{U}_{m-2}\| \leq K[\|p\|_{L^\infty(H^{k+1})}, \|u\|_{L^\infty(H^{k+1}(\mathrm{div}))}]h_p^{k+1}\,, \tag{4.8}$$

and that by (3.9) and (2.5),

$$\begin{aligned}\|E\tilde{U}^n - EU^n\| &\leq K\|c_{m-1} - C_{m-1}\| + K\|c_{m-2} - C_{m-2}\| \\ &\leq K\|\xi_{m-1}\| + K\|\xi_{m-2}\| + K\|\zeta_{m-1}\| + K\|\zeta_{m-2}\| \\ &\leq K[\|c\|_{L^\infty(H^{l+1})}]h_c^{l+1} + K\|\zeta_{m-1}\| + K\|\zeta_{m-2}\| .\end{aligned} \tag{4.9}$$

Thus, using (4.8), (4.9) and the estimate in (4.7),

$$\begin{aligned}|T_3| &\leq K[\|u^n - Eu^n\| + \|Eu^n - E\tilde{U}^n\| + \|E\tilde{U}^n - EU^n\|]\|\nabla\tilde{C}^n\|_{L^\infty}\|\nabla\zeta^n\| \\ &\leq K(\Delta t_p)^3 \left\| \frac{\partial^2 u}{\partial t^2} \right\|^2_{L^2(t_{m-2},\, t_m;\, L^2)} + K[\|p\|_{L^\infty(H^{k+1})}, \|u\|_{L^\infty(H^{k+1}(\mathrm{div}))}]h_p^{2k+2} \\ &\quad + K[\|c\|_{L^\infty(H^{l+1})}]h_c^{2l+2} + K\|\zeta_{m-1}\|^2 + K\|\zeta_{m-2}\|^2 + \varepsilon\|\nabla\zeta^n\|^2 .\end{aligned} \tag{4.10}$$

The remark after (4.7) about the temporal error term applies here as well.

By (2.6), we have

$$\begin{aligned}|T_4| &\leq K\left\| \frac{\xi^n - \xi^{n-1}}{\Delta t_c} \right\|^2 + K\|\zeta^n\|^2 \leq K(\Delta t_c)^{-1} \left\| \frac{\partial \xi}{\partial t} \right\|^2_{L^2(t^{n-1},\, t^n;\, L^2)} + K\|\zeta^n\|^2 \\ &\leq K(\Delta t_c)^{-1} h_c^{2l+2} \|c\|^2_{H^1(t^{n-1},\, t^n;\, H^{l+1})} + K\|\zeta^n\|^2 ,\end{aligned} \tag{4.11}$$

and (2.5) yields at once

$$\begin{aligned}|T_5| &\leq K[\|c\|_{L^\infty(H^{l+1})}]h_c^{2l+2} + K\|\zeta^n\|^2 , \\ |T_6| &\leq K\|\zeta^n\|^2 .\end{aligned} \tag{4.12}$$

The estimates of T_7, T_8 and T_9 fit into the following general picture. Let f be defined on Ω; in the three estimates, f will be c, ξ and ζ, respectively. Let z denote the unit vector in the direction of $EU^n - Eu^n$. Then

$$\begin{aligned}\int_\Omega \phi \frac{\hat{f}^{n-1} - \check{f}^{n-1}}{\Delta t_c} \zeta^n \, dx &= (\Delta t_c)^{-1} \int_\Omega \phi \left[\int_{\check{x}}^{\hat{x}} \frac{\partial f^{n-1}}{\partial z} dz \right] \zeta^n \, dx \\ &= (\Delta t_c)^{-1} \int_\Omega \phi \left[\int_0^1 \frac{\partial f^{n-1}}{\partial z} ((1-\bar{z})\check{x} + \bar{z}\hat{x}) \, d\bar{z} \right] |\hat{x} - \check{x}| \zeta^n \, dx \\ &= \int_\Omega \left[\int_0^1 \frac{\partial f^{n-1}}{\partial z} ((1-\bar{z})\check{x} + \bar{z}\hat{x}) \, d\bar{z} \right] |E(u-U)^n| \zeta^n \, dx ,\end{aligned} \tag{4.13}$$

where $\bar{z} \in [0, 1]$ parametrizes the segment from $\check{x}$ to $\hat{x}$ and we have used the fact that $\hat{x} - \check{x} = \Delta t_c[Eu^n(x) - EU^n(x)]/\phi(x)$. Let

$$g_f(x) = \int_0^1 \frac{\partial f^{n-1}}{\partial z} ((1-\bar{z})\check{x} + \bar{z}\hat{x}) \, d\bar{z} ;$$

then we can write three special cases of (4.13),

$$\begin{aligned}|T_7| &\leq \|g_c\|_{L^\infty}\|E(u-U)^n\|\|\zeta^n\|,\\ |T_8| &\leq \|g_\xi\|\|E(u-U)^n\|\|\zeta^n\|_{L^\infty},\\ |T_9| &\leq \|g_\zeta\|\|E(u-U)^n\|\|\zeta^n\|_{L^\infty}.\end{aligned} \tag{4.14}$$

In the T_3 estimate, we showed that

$$\|E(u-U)^n\|^2 \leq Kh_{\mathrm{p}}^{2k+2} + Kh_{\mathrm{c}}^{2l+2} + K\|\zeta_{m-1}\|^2 + K\|\zeta_{m-2}\|^2. \tag{4.15}$$

Since $g_c(x)$ is an average of certain first partial derivatives of c^{n-1}, which are bounded by $\|c^{n-1}\|_{W_\infty^1}$, (4.14) leads to

$$|T_7| \leq K\|E(u-U)^n\|^2 + K\|\zeta^n\|^2. \tag{4.16}$$

To bound $\|g_\xi\|$ and $\|g_\zeta\|$, we require an induction hypothesis. Assume that

$$\|U_{m-i}\|_{L^\infty} \leq \left[\frac{h_{\mathrm{p}}}{\Delta t_{\mathrm{c}}}\right]^{1/2}, \quad i = 1, 2. \tag{4.17}$$

If concentration time level t^n coincides with pressure level t_m, we verify (4.17) for U_m at the end of the proof. Now note that

$$\|g_f\|^2 \leq \int_0^1 \int_\Omega \left| \frac{\partial f^{n-1}}{\partial z}((1-\bar{z})\check{x} + \bar{z}\hat{x})\right|^2 \mathrm{d}x\, \mathrm{d}\bar{z}. \tag{4.18}$$

Define the transformation

$$G_{\bar{z}}(x) = (1-\bar{z})\check{x} + \bar{z}\hat{x} = x - \left[\frac{Eu^n(x)}{\phi(x)} + \bar{z}\,\frac{E(U-u)^n(x)}{\phi(x)}\right]\Delta t_{\mathrm{c}}. \tag{4.19}$$

Letting $\mathcal{T}$ run over the elements in the pressure mesh, (4.18) becomes

$$\|g_f\|^2 \leq \int_0^1 \sum_{\mathcal{T}} \int_{\mathcal{T}} \left| \frac{\partial f^{n-1}}{\partial z}(G_{\bar{z}}(x))\right|^2 \mathrm{d}x\, \mathrm{d}\bar{z}. \tag{4.20}$$

The Jacobian of $G_{\bar{z}}$ is the identity matrix, plus Δt_{c} times terms involving first partial derivatives of ϕ and Eu (which are bounded) and of EU (which exist on each $\mathcal{T}$; U is discontinuous at pressure mesh edges). On each $\mathcal{T}$, the $\nabla(EU)\Delta t_{\mathrm{c}}$ terms can be bounded by ($\mathrm{I_p}$) and (4.17),

$$|\nabla(EU)|\Delta t_{\mathrm{c}} \leq Kh_{\mathrm{p}}^{-1}\|U_{m-i}\|_{L^\infty}\Delta t_{\mathrm{c}} \leq K\left[\frac{\Delta t_{\mathrm{c}}}{h_{\mathrm{p}}}\right]^{1/2} = \mathrm{o}(1), \tag{4.21}$$

since $\Delta t_{\mathrm{c}} = \mathrm{o}(h_{\mathrm{p}})$. Thus

$$\det DG_{\bar{z}} = 1 + \mathrm{o}(1)\,. \tag{4.22}$$

Changing variables in (4.20), it then follows that

$$\|g_f\|^2 \leqslant 2 \int_0^1 \sum_{\mathcal{T}} \int_{G_{\bar{z}}(\mathcal{T})} \left| \frac{\partial f^{n-1}}{\partial z}(x) \right|^2 \mathrm{d}x\, \mathrm{d}\bar{z}\,. \tag{4.23}$$

We also see that $G_{\bar{z}}$ is a one-to-one mapping on each $\mathcal{T}$, because (4.19) and (4.21) imply that

$$\begin{aligned} |G_{\bar{z}}(x) - G_{\bar{z}}(x')| &\geqslant |x - x'|[1 - K\Delta t_{\mathrm{c}} \|\nabla(EU)\|_{L^\infty(\mathcal{T})}] \\ &= |x - x'|(1 - \mathrm{o}(1))\,; \end{aligned} \tag{4.24}$$

furthermore, $G_{\bar{z}}$ maps $\mathcal{T}$ into itself and its immediate-neighbor elements, since

$$\begin{aligned} |G_{\bar{z}}(x) - x| &= \Delta t_{\mathrm{c}} \left[\mathrm{O}(1) + \mathrm{O}\left[\left[\frac{h_{\mathrm{p}}}{\Delta t_{\mathrm{c}}}\right]^{1/2}\right]\right] \\ &= \mathrm{O}(\Delta t_{\mathrm{c}}) + \mathrm{O}[h_{\mathrm{p}}^{1/2} \Delta t_{\mathrm{c}}^{1/2}] \\ &= \mathrm{o}(h_{\mathrm{p}})\,. \end{aligned} \tag{4.25}$$

Hence, $G_{\bar{z}}$ is globally at most finitely-many-to-one (with repetition factor bounded by the number of neighbors of an element) and maps Ω into itself and its immediate-neighbor periodic copies. This implies that the sum in (4.23) is bounded by finitely many multiples of an Ω-integral, so that

$$\|g_f\|^2 \leqslant K \|\nabla f^{n-1}\|^2\,. \tag{4.26}$$

We now apply (4.26) to (4.14) and use an argument of Douglas [5]. Douglas cites a theorem of Bramble [1] which, since ζ^n is a test function in two dimensions, implies that

$$\|\zeta^n\|_{L^\infty} \leqslant K |\log h_{\mathrm{c}}|^{1/2} \|\zeta^n\|_1\,. \tag{4.27}$$

By (4.14), (4.26), (4.27) and (2.5), we have

$$\begin{aligned} |T_8| &\leqslant K \|\nabla \xi^{n-1}\| \|E(u - U)^n\| |\log h_{\mathrm{c}}|^{1/2} \|\zeta^n\|_1 \\ &\leqslant K h_{\mathrm{c}}^{2l} |\log h_{\mathrm{c}}| \, \|E(u - U)^n\|^2 + \varepsilon \|\zeta^n\|_1^2 \\ &\leqslant K \|E(u - U)^n\|^2 + \varepsilon \|\zeta^n\|_1^2\,. \end{aligned} \tag{4.28}$$

From (4.15), it is clear that $\|E(u - U)^n\| = \mathrm{o}(|\log h_{\mathrm{c}}|^{-1/2})$, since our theorem will prove (inductively) that $\|\zeta_{m-i}\| = \mathrm{O}[h_{\mathrm{c}}^{l+1} + h_{\mathrm{p}}^{k+1} + \Delta t_{\mathrm{c}} + (\Delta t_{\mathrm{p}}^1)^{3/2} + (\Delta t_{\mathrm{p}})^2]$. Thus, emulating (4.28),

$$\begin{aligned} |T_9| &\leqslant K \|E(u - U)^n\| |\log h_{\mathrm{c}}|^{1/2} \|\zeta^n\|_1^2 \\ &\leqslant \varepsilon \|\zeta^n\|_1^2\,. \end{aligned} \tag{4.29}$$

Combining (4.15), (4.16), (4.28) and (4.29), we have

$$|T_7|+|T_8|+|T_9|\leq Kh_{\mathrm{p}}^{2k+2}+Kh_{\mathrm{c}}^{2l+2}+K\|\zeta_{m-1}\|^2+K\|\zeta_{m-2}\|^2+K\|\zeta^n\|^2+\varepsilon\|\zeta^n\|_1^2\,. \tag{4.30}$$

Before estimating T_{10}, we examine (4.13). The difference $(\hat{f}^{n-1}-\check{f}^{n-1})/\Delta t_c$ behaved like a *spatial* derivative of f times $|\hat{x}-\check{x}|/\Delta t_c$. Similarly, we expect $(\xi^{n-1}-\check{\xi}^{n-1})/\Delta t_c$ in T_{10} to be like a spatial derivative of ξ times $|x-\check{x}|/\Delta t_c=|Eu^n(x)|/\phi(x)=\mathrm{O}(1)$. To obtain an optimal $(\mathrm{O}(h_c^{l+1}))$ L^2 error estimate, we must therefore use an H^{-1} norm on $(\xi^{n-1}-\check{\xi}^{n-1})/\Delta t_c$ and an H^1 norm on the function $\phi\zeta^n$. We have

$$\left\|\frac{\xi^{n-1}-\check{\xi}^{n-1}}{\Delta t_c}\right\|_{-1}=\frac{1}{\Delta t_c}\sup_{f\in H^1}\left[\frac{1}{\|f\|_1}\int_\Omega[\xi^{n-1}(x)-\xi^{n-1}(\check{x})]f(x)\,\mathrm{d}x\right]. \tag{4.31}$$

Set

$$G(x)=\check{x}=x-\frac{Eu^n(x)}{\phi(x)}\Delta t_c\,;$$

by periodicity, G may be considered as a differentiable mapping of Ω into itself. We claim that G is in fact a differentiable homeomorphism of Ω onto itself.

First we note that analogues of (4.22), (4.24), and (4.25), with $\mathrm{O}(\Delta t_c)$ in place of $\mathrm{o}(1)$ and $\mathrm{o}(h_p)$, hold for G; they are easier to demonstrate, since U is not involved and G is smooth. It follows from the analogue of (4.22) and the inverse function theorem that G is locally a differentiable homeomorphism onto its image, and the analogue of (4.24) shows that G is globally one-to-one. Since $\bar{\Omega}$ is compact, G is a closed one-to-one mapping of $\bar{\Omega}$ and is therefore globally a homeomorphism onto its image. It remains only to show that G is onto. Let $\tilde{\Omega}$ be the union of Ω and its neighboring periodic copies, and suppose that there exists $x_0\in\Omega$ such that $x_0\notin G(\tilde{\Omega})$. Let Γ be a loop in $\tilde{\Omega}$ wrapping around x_0 at distance greater than $\|Eu^n/\phi\|_{L^\infty}\Delta t_c$ from x_0 and $\partial\tilde{\Omega}$. By the G-analogue of (4.25), $G(\Gamma)$ still wraps around $x_0\notin G(\tilde{\Omega})$. But $G(\tilde{\Omega})$ is simply connected since $\tilde{\Omega}$ is, so we have a contradiction. This proves the claim.

Thus, we can change variables in (4.31) and write

$$\begin{aligned}\left\|\frac{\xi^{n-1}-\check{\xi}^{n-1}}{\Delta t_c}\right\|_{-1}&=\frac{1}{\Delta t_c}\sup_{f\in H^1}\left(\frac{1}{\|f\|_1}\left[\int_\Omega\xi^{n-1}(x)f(x)\,\mathrm{d}x\right.\right.\\&\qquad\left.\left.-\int_\Omega\xi^{n-1}(x)f(G^{-1}(x))\det DG(x)^{-1}\,\mathrm{d}x\right]\right)\\&\leq\frac{1}{\Delta t_c}\sup_{f\in H^1}\left[\frac{1}{\|f\|_1}\int_\Omega\xi^{n-1}(x)f(x)[1-\det DG(x)^{-1}]\,\mathrm{d}x\right]\\&\quad+\frac{1}{\Delta t_c}\sup_{f\in H^1}\left[\frac{1}{\|f\|_1}\int_\Omega\xi^{n-1}(x)[f(x)-f(G^{-1}(x))]\det DG(x)^{-1}\,\mathrm{d}x\right]\\&\equiv W_1+W_2\,.\end{aligned} \tag{4.32}$$

The G-analogue of (4.22), with $\mathrm{O}(\Delta t_c)$ instead of $\mathrm{o}(1)$, yields

$$|W_1| \leq K \sup_{f\in H^1} [\|\xi^{n-1}\| \|f\| / \|f\|_1] \leq K\|\xi^{n-1}\| . \tag{4.33}$$

A bound for det $DG(x)^{-1}$ and an argument like (4.13) lead to

$$|W_2| \leq \frac{2}{\Delta t_c} \sup_{f\in H^1} \left[\frac{1}{\|f\|_1} \int_\Omega \xi^{n-1}(x) g_f^*(x) |x - G^{-1}(x)| \, dx\right], \tag{4.34}$$

where

$$g_f^*(x) = \int_0^1 \frac{\partial f}{\partial z^*}((1-\bar{z}^*)G^{-1}(x) + \bar{z}^* x) \, d\bar{z}^*$$

and z^* is the unit vector in the direction of $x - G^{-1}(x)$. By the G-analogue of (4.25), we have

$$|x - G^{-1}(x)| \leq K \Delta t_c . \tag{4.35}$$

Since G^{-1} is continuous and differentiable, a simpler global version of the argument leading to (4.26) tells us that

$$\|g_f^*\| \leq K\|f\|_1 . \tag{4.36}$$

Combining (4.34), (4.35) and (4.36), we have

$$|W_2| \leq K\|\xi^{n-1}\| . \tag{4.37}$$

By (4.32), (4.33), (4.37) and (2.5), we have the estimate

$$|T_{10}| \leq K h_c^{2l+2} + \varepsilon \|\zeta^n\|_1^2 . \tag{4.38}$$

The same argument gives

$$|T_{11}| \leq K\|\zeta^{n-1}\|^2 + \varepsilon \|\zeta^n\|_1^2 . \tag{4.39}$$

We now combine (4.3) with the estimates (4.6), (4.7), (4.10), (4.11), (4.12), (4.30), (4.38) and (4.39) to see that

$$\begin{aligned}
&\frac{1}{2\Delta t_c}[(\phi\zeta^n, \zeta^n) - (\phi\zeta^{n-1}, \zeta^{n-1})] + (D(EU^n)\nabla\zeta^n, \nabla\zeta^n) \leq \\
&\quad \leq K(\|c\|_{L^\infty(H^{l+1})}) h_c^{2l+2} + K\|c\|_{H^1(t^{n-1}, t^n; H^{l+1})}^2 h_c^{2l+2} (\Delta t_c)^{-1} \\
&\qquad + K(\|p\|_{L^\infty(H^{k+1})}, \|u\|_{L^\infty(H^{k+1}(\mathrm{div}))}) h_p^{2k+2} \\
&\qquad + K\left\|\frac{\partial^2 c}{\partial \tau^2}\right\|_{L^2(t^{n-1}, t^n; L^2)}^2 \Delta t_c + K\left\|\frac{\partial^2 u}{\partial t^2}\right\|_{L^2(t_{m-2}, t_m; L^2)}^2 (\Delta t_p)^3 \\
&\qquad + K\|\zeta^n\|^2 + K\|\zeta^{n-1}\|^2 + K\|\zeta_{m-1}\|^2 + K\|\zeta_{m-2}\|^2 + \varepsilon\|\nabla\zeta^n\|^2 .
\end{aligned} \tag{4.40}$$

If $t^n \leq t_1$, the remark after (4.7) applies. Multiply (4.40) by Δt_c and sum on n, noting that the $(\Delta t_p)^3$, ζ_{m-1} and ζ_{m-2} terms repeat $\Delta t_p/\Delta t_c$ times and that the $(\Delta t_p^1)^2$ term of the remark after (4.7) repeats $\Delta t_p^1/\Delta t_c$ times. The ε term hides on the left-hand side of (4.40), and the ζ terms disappear by the discrete Gronwall lemma (with an obvious generalization to cover the $\sum \|\zeta_m\|^2 \Delta t_p$ term) at the cost of a multiplicative constant. Since $\zeta^0 = 0$, we obtain

$$\max_n \|\zeta^n\|^2 + \sum_n \|\nabla \zeta^n\|^2 \Delta t_c \leq K(h_c^{2l+2} + h_p^{2k+2} + (\Delta t_c)^2 + (\Delta t_p^1)^3 + (\Delta t_p)^4), \tag{4.41}$$

from which (4.1) follows at once.

It remains to check the induction hypothesis (4.17), if $t^n = t_m$. We have, by (3.7), (I_p), (3.9), (2.5) and (4.41), that

$$\begin{aligned} \|U_m\|_{L^\infty} &\leq \|\tilde{U}_m\|_{L^\infty} + \|U_m - \tilde{U}_m\|_{L^\infty} \\ &\leq K + Kh_p^{-1}\|U_m - \tilde{U}_m\| \\ &\leq K + Kh_p^{-1}\|c_m - C_m\| \\ &\leq K + Kh_p^{-1}(\|\xi^n\| + \|\zeta^n\|) \\ &\leq K + Kh_p^{-1}[h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p^1)^{3/2} + (\Delta t_p)^2] \\ &\leq \left[\frac{h_p}{\Delta t_c}\right]^{1/2} \end{aligned} \tag{4.42}$$

for h_p sufficiently small, since $\Delta t_c = o(h_p)$ and the other terms in parentheses are $O(h_p)$. This completes the proof. □

By combining Theorem 4.1 with (3.6) and (3.9), we obtain at once the following result.

COROLLARY 4.2. Under the assumptions of Theorem 4.1, *the errors in velocity and pressure are bounded by*

$$\max_m(\|u_m - U_m\|_{H(\mathrm{div};\,\Omega)} + \|p_m - P_m\|) \leq K[h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p^1)^{3/2} + (\Delta t_p)^2]\,.$$

Extensions and remarks. Of the mesh restrictions in Theorem 4.1, the only significant one is $\Delta t_c = o(h_p)$, and it is important only in the case $k = 0$. We would prefer to be able to choose $\Delta t_c = O(h_p)$ in that case. If the pressure mesh is uniform, this minor difficulty can be circumvented with a postprocessing method of Douglas [7]. In that work, the computed velocity U is convolved with a Bramble–Schatz kernel [2, 3] that takes advantage of superconvergent points to double the global order of accuracy in h_p. It is clear that the proof of Theorem 4.1 would go through with this higher order, so that the requirement $\Delta t_c = o(h_p)$ would become insignificant even when $k = 0$.

As we noted after (4.6), the modified method of characteristics reduces the time-truncation error of standard procedures. We see also in (4.40) that the mixed method causes most error terms that would otherwise be pressure-dependent to depend on norms of the velocity, which is a smoother function. Numerical computations [13] have shown that this combination of methods can use long time steps; the approximations improve over those of standard schemes from the viewpoints of stability, rotation invariance, and avoidance of numerical dispersion.

It is possible to obtain an optimal-order error estimate in $H^1(\Omega)$ by using the test function $(\zeta^n - \zeta^{n-1})/\Delta t_c$ in (4.2). The proof is a straightforward modification of the proof of Theorem 4.1 if the diffusion-dispersion coefficient D is independent of velocity (i.e., if it represents molecular diffusion only). In the velocity-dependent case considered here, a lengthy argument based on summation by parts in time is necessary to handle the analogue of T_3 in Theorem 4.1. It is also possible to incorporate into the analysis an approximate solution of the algebraic equations, such as preconditioned conjugate-gradient iteration, at each time step. The techniques needed to analyze these extensions have appeared in [12, 17].

It should also be possible to extend the results to three space dimensions. To obtain (2.7) and (3.7), we would have to assume $c \in L^\infty(H^3)$, $p \in L^\infty(H^2)$, and $u \in L^\infty(H^2(\mathrm{div}))$. We would have to replace h_p^{-1} by $h_p^{-3/2}$ in (4.42), $\Delta t_c = o(h_p)$ by $\Delta t_c = o(h_p^{3/2})$ in Theorem 4.1, and $(h_p/\Delta t_c)^{1/2}$ by $h_p^{-1/2}[h_p^{3/2}/\Delta t_c]^{1/2}$ in (4.17). Then (4.21), as modified, would still hold. Assuming that (4.27) could be replaced by $O[h_c^{-1/2}|\log h_c|\,\|\zeta^n\|_1]$, we would replace $2l$ by $2l-1$ in (4.28) and the entire proof would still go through. The tightened restriction $\Delta t_c = o(h_p^{3/2})$ would be serious when $k = 0$, making the postprocessing procedure mentioned above potentially useful in that case.

Acknowledgment

Much of this work traces back to ideas of Jim Douglas, Jr., who has influenced all of the authors greatly. The second author thanks the management of Marathon Oil Company for permission to publish this paper. The first author is supported in part by the U.S. Army Research Office.

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