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A TIME-DISCRETIZATION PROCEDURE
FOR A MIXED FINITE ELEMENT APPROXIMATION
OF MISCIBLE DISPLACEMENT IN POROUS MEDIA (*)

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Abstract. — *An efficient time-stepping procedure is introduced to treat the continuous-time method of the authors which employs a mixed finite element method to approximate the pressure and the fluid velocity and a standard Galerkin method to approximate the concentration for the system describing the miscible displacement of one incompressible fluid by another in a porous medium. The concentration equations are solved by Gaussian elimination at each concentration time level, but the number of matrix factorizations is reduced to one per pressure time step, which is much larger than the concentration time step. Optimal order error estimates are derived under certain constraints between the discretization parameters. It is shown that the natural choices for these parameters satisfy the constraints with the exception of one case, for which a very mild pressure time step restriction is introduced.*

Résumé. — *On introduit un procédé efficace de discrétisation en temps pour traiter la méthode (continue en temps) des auteurs, qui utilise une méthode d'éléments finis mixtes pour approcher la pression et la vitesse du fluide ainsi qu'une méthode classique de Galerkin pour approcher la concentration, dans un système décrivant le déplacement miscible d'un fluide incompressible par un autre dans un milieu poreux. On résout les équations de concentration par élimination de Gauss à chaque niveau de temps en concentration, mais le nombre de factorisations matricielles est réduit à un par niveau de temps en pression, qui est beaucoup plus grand que le pas de temps en concentration. On obtient des ordres optimaux pour les estimations d'erreur lorsque certaines relations sont vérifiées par les paramètres de discrétisation. On montre que les choix naturels pour ces paramètres satisfont ces relations sauf dans un cas, où une restriction très faible sur le pas de temps en pression est introduite.*

1. INTRODUCTION

The miscible displacement of one incompressible fluid by another in a porous medium $\Omega \subset R^2$ of unit thickness and nonuniform local elevation can be described by a differential system that can be put in the form [7, 9, 10]

$$(a) \quad \nabla . u = - \sum_{i=1}^{2} \frac{\partial}{\partial x_i} \left[a_i(x, c) \left(\frac{\partial p}{\partial x_i} - \gamma_i(x, c) \right) \right] = q ,$$

$$(b) \quad \phi(x) \frac{\partial c}{\partial t} + u.\nabla c - \nabla.(D \nabla c) = (\tilde{c} - c) q = g(x, t, c) ,$$

(1:1)

for $x \in \Omega$ and $t \in J = [0, T]$, where the diffusion coefficient $D = D(x, u)$ is the 2×2 matrix given by

$$D = \phi(x) \{ d_m I + | u | (d_l E(u) + d_t E^\perp(u)) \},$$ (1.2)

with $e_{ij}(u) = u_i u_j/| u |^2$ and $E^\perp = I - E$. We impose the boundary conditions

$$(a) \qquad\qquad u.v = 0,$$

$$(b) \quad \sum_{i,j=1}^{2} D_{ij}(x, u) \frac{\partial c}{\partial x_i} v_j = 0$$ (1.3)

on $\partial\Omega \times J$, where v is the outer normal to Ω; for compatibility (i.e., incompressibility)

$$(q, 1) = \int_\Omega q \, dx = 0, \qquad t \in J.$$ (1.4)

The initial concentration

$$c(x, 0) = c_0(x)$$ (1.5)

must be specified, and the initial pressure can then be determined from (1.1a) and (1.3a).

The authors [4] have previously defined a continuous-time finite element method based on the use of an elliptic mixed finite element method to approximate the pressure p and the velocity u and a parabolic Galerkin method to approximate the concentration c. It is particularly suitable to employ the mixed method, since only the velocity and not the pressure appears in the concentration equation. The object of this paper is to discuss a time-stepping procedure for the finite element procedure that efficiently reflects the fact that the velocity field varies slower in time than either the concentration or the pressure for reasonable physical data. Thus, we shall take the pressure time step to be much larger than the concentration time step. We shall consider a procedure that is based on the direct solution of linear equations for the concentration at each concentration time level; the matrices and equations arising for each step will be modified so that only one factorization will be required for each pressure time step, rather than each concentration step. The modification will be made in such a way that the asymptotic order of convergence is unaffected. We shall consider the algebraic equations for the approximate pressure to be solved exactly.

Other time-stepping methods have been discussed for various finite difference and finite element methods for the miscible displacement problem. In particular, the concept of time-stepping nonlinear parabolic equations by incomplete iteration [3] has been extended [6, 12] to certain finite element procedures for the miscible problem. The method of this paper is in a sense an outgrowth of a refinement [1] of an efficient direct solution method [2] for nonlinear parabolic equations; a variant of it has been applied [5] experimentally.

Since this paper is a continuation of the authors' paper [4], we shall use the same notation as far as possible and we shall make use of the results of that paper wherever feasible to shorten our arguments here. An outline of this paper is as follows. The continuous-time method of [4] will be recalled, and then the time-discretization procedure will be derived. Some technical results to be used in the convergence analysis will be summarized, and then the demonstration of the convergence of the fully discrete method will be given. The finite element spaces for the pressure and the concentrations will be allowed to be associated with different polygonalizations of the domain, and the time step for the pressure will be taken larger than that for the concentration. Optimal order error estimates will be obtained under certain constraints on the discretization parameter. Finally, it will be shown that these constraints are natural and pose no practical difficulty.

2. FORMULATION OF THE METHOD

Let

$$
\begin{aligned}
&(a) \quad V = H(\mathrm{div}\,;\Omega) \cap \{\, v.\mathrm{v} = 0 \text{ on } \partial\Omega \,\}, \\
&(b) \quad W = L^2(\Omega)/\{\, \varphi \equiv \text{constant on } \Omega \,\},
\end{aligned}
\tag{2.1}
$$

and set

$$
\begin{aligned}
&(a) \quad A(\theta\,;\alpha,\beta) = \left(\frac{1}{a(\theta)}\,\alpha, \beta\right) = \sum_{i=1}^{2}\left(\frac{1}{a_i(\theta)}\,\alpha_i, \beta_i\right), \\
&(b) \qquad B(\alpha, \varphi) = -(\mathrm{div}\,\alpha, \varphi)
\end{aligned}
\tag{2.2}
$$

for $\alpha,\ \beta \in V$, $\varphi \in W$, and $\theta \in L^\infty(\Omega)$. The pressure equation is equivalent to the saddlepoint problem

$$
\begin{aligned}
&(a) \quad A(c\,;u,v) + B(v,p) = (\gamma(c), v), \qquad v \in V, \\
&(b) \qquad\qquad B(u, \varphi) = -(q, \varphi), \qquad \varphi \in W,
\end{aligned}
\tag{2.3}
$$

at each time $t \in J$. The concentration equation is equivalent to finding a diffe-
rentiable map $c : J \to H^1(\Omega)$ such that

$$\left(\phi \frac{\partial c}{\partial t}, z \right) + (u.\nabla c, z) + (D(u) \nabla c, \nabla z) = (g(c), z) \qquad (2.4)$$

for $z \in H^1(\Omega)$ and $0 < t \leqslant T$ and such that $c(x, 0) = c_0(x)$.

Let $h = (h_c, h_p)$, with h_c and h_p being positive. Assume that Ω is a poly-
gonal domain and that $\tilde{V}_h \times \tilde{W}_h$ is a Raviart-Thomas space [11] of index k
associated with a quasi-regular triangulation or quadrilateralization of Ω
such that the elements have diameters bounded by h_p. (The argument below
covers the case of the extension to curvilinear boundary elements given by
Johnson and Thomée [8] for the index $k = 1$.) Set

$$(a) \quad V_h = \{ v \in \tilde{V}_h : v.\nu = 0 \text{ on } \partial\Omega \},$$
$$(b) \quad W_h = \tilde{W}_h/\{ \varphi \equiv \text{constant on } \Omega \}. \qquad (2.5)$$

The approximation properties of $V_h \times W_h$ are given by the relations (3.2)
of [4]. Then, let $M_h \subset H^1(\Omega)$ be a standard finite element space for a Galerkin
method, and assume that it is associated with a quasi-regular polygonaliza-
tion of Ω and that it is of index l :

$$\inf_{z_h \in M_h} \| z - z_h \|_{H^1(\Omega)} \leqslant M \| z \|_{H^{l+1}(\Omega)} h_c^l. \qquad (2.6)$$

Let

$$(a) \quad \Delta t_c > 0, \qquad t_c^n = n \Delta t_c,$$
$$(b) \quad \Delta t_p = Q \Delta t_c, \qquad Q \in Z^+, \qquad t_p^m = m \Delta t_p. \qquad (2.7)$$

The multiplier Q will, in general, depend on Δt_c. The algorithm will be describ-
ed so as to advance the solution one pressure time step. First, approximate
c_0 by a function $C^0 = C(t_c^0) \in M_h$; this can be done by interpolation, by
L^2-projection, or by projection with respect to some Dirichlet form.

Now, assume $C(t_p^m)$ known. Then, the velocity-pressure pair $\{ U^m, P^m \}$
at time t_p^m can be calculated as the (mixed method) solution of the system

$$(a) \quad A(C(t_p^m); U^m, v) + B(v, P^m) = (\gamma(C(t_p^m)), v), \qquad v \in V_h,$$
$$(b) \qquad\qquad\qquad B(U^m, \varphi) = -(q(t_p^m), \varphi), \qquad \varphi \in W_h. \qquad (2.8)$$

The question at hand is to discretize the concentration equation in time for
$t_p^m < t_c^n \leqslant t_p^{m+1}$. This will be done by deriving, thorough several stages, a
convenient variant of a backward-differenced Galerkin procedure.

The standard backward-difference equation would be of the form

$$\left(\phi \, \frac{C^n - C^{n-1}}{\Delta t_c} , z \right) + (U(t_c^n) . \nabla C^n, z)$$

$$+ (D(U(t_c^n)) \, \nabla C^n, \nabla z) = (g(C^n), z), \qquad z \in M_h, \qquad (2.9)$$

where $C^n = C(t_c^n) \in M_h$. Since $t_c^n \notin \{ t_p^j : j = 0, ..., m \}$, we have no values for the velocity $U(t_c^n)$ available directly from a pressure calculation. For $m \geqslant 1$, this difficulty can easily be eliminated by linear extrapolation. Set

$$\overline{U}^n = \frac{t_c^n - t_p^{m-1}}{t_p^m - t_p^{m-1}} \, U^m - \frac{t_c^n - t_p^m}{t_p^m - t_p^{m-1}} \, U^{m-1} \qquad (2.10)$$

for $t_p^m < t_c^n \leqslant t_p^{m+1}$ and replace $U(t_c^n)$ by $\overline{U}^n$ in (2.9). For $m = 0$, first use $\overline{U}^n = U^0$, then use (2.8) to obtain a first estimate to U^1, then rework the first pressure step using interpolation for $\overline{U}^n$ between U^0 and the estimated U^1, and then continue as above; i.e., use a predictor-corrector concept for one pressure step. It can be helpful to correct twice. (In practice, it is often feasible and desirable to utilize an asymptotic solution for the concentration at early time, so that this predictor-corrector step can be avoided; see [5].)

Next, there is the possibility of nonlinearity in the algebraic system (2.9) arising from the appearance of $g(C^n)$. If $g(c)$ is linear, as it is for practical purposes when g has the form $g(c) = (\tilde{c} - c) q$ as in (1.1b), then no modification of this term is necessary. If not, then since we are expecting only first-order convergence in Δt_c as a result of the discretization of $\partial c / \partial t$, we can extrapolate C^{n-1} and C^{n-2} in the evaluation of $g(C^n)$. Set

$$\check{C}^n = \begin{cases} C^n, & \text{if } g(C) = \alpha C + \beta, \\ 2 \, C^{n-1} - C^{n-2}, & \text{otherwise} \end{cases} \qquad (2.11)$$

and replace $g(C^n)$ by $g(\check{C}_n)$. At this point, we are looking at the equations

$$\left(\phi \, \frac{C^n - C^{n-1}}{\Delta t_c} , z \right) + (\overline{U}^n . \nabla C^n, z) + (D(\overline{U}^n) \, \nabla C^n, \nabla z) = (g(\check{C}^n), z), \quad z \in M_h .$$

$$(2.12)$$

Let us turn our attention to the computational aspects of solving (2.12). Let

$$M_h = \text{Span} \{ z_1, ..., z_N \} \qquad (2.13)$$

and form the matrices

$$(a) \quad \mathscr{C} = [(\phi z_j, z_i)],$$

$$(b) \quad \mathscr{A}^n = \mathscr{A}(\overline{U}^n) = [(\overline{U}^n.\nabla z_j, z_i) + (D(\overline{U}^n)\nabla z_j, \nabla z_i)].$$
(2.14)

Let $\psi_i^n = (g(\check{C}^n), z_i)$ and $\psi^n = (\psi_1^n, ..., \psi_N^n)^T$, where for simplicity in the discussion we are going to assume the « otherwise » case in the evaluation of C^n from here on ; the linear case is slightly easier to treat in the analysis and has no noticeable effect on the computational complexity discussion. In matricial form (2.12) becomes

$$(\mathscr{C} + \Delta t_c \mathscr{A}^n) \beta^n = \mathscr{C}\beta^{n-1} + \Delta t_c \psi^n,$$
(2.15)

where

$$C^n = \sum_{i=1}^{N} \beta_i^n z_i.$$
(2.16)

If a good sparse matrix procedure that takes proper account of the structure of $\mathscr{C} + \Delta t_c \mathscr{A}^n$ is used, then the operation counts for the LU-factorization, the forward and backward solutions of $LU\beta = \tilde{\psi}$, and the formation of the matrices and the right-hand side are as follows :

(i)   Formation of $\mathscr{C} + \Delta t_c \mathscr{A}^n$ $O(N)$

(ii) Formation of $\mathscr{C}\beta^{n-1} + \Delta t_c \psi^n = \tilde{\psi}^n$ $O(N)$

(iii) Factorization of $\mathscr{C} + \Delta t_c \mathscr{A}^n$ $O(N^{3/2})$ (2.17)

(iv) Solution of $LU\beta^n = \tilde{\psi}^n$ $O(N \log N).$

Thus, the calculation is dominated by the factorization, and it would be very advantageous to reduce significantly the number of factorizations. The final modification of (2.9) or (2.12) presents a method requiring a single factorization of a matrix of the form $\mathscr{C} + \Delta t_c \mathscr{A}(U)$ over each pressure time step, instead of one each concentration step.

Recall that p and u are approximated by equations having no explicit dependence on the time ; hence, linear extrapolation of U can be hoped to produce second-order accuracy in the pressure time step. Set

$$\overline{U}_p^{m+1/2} = \frac{3}{2} U^m - \frac{1}{2} U^{m-1}.$$
(2.18)

Finally, consider the relation

$$\left(\phi \frac{C^n - C^{n-1}}{\Delta t_c}, z\right) + (\overline{U}_p^{m+1/2}.\nabla C^n, z) + (D(\overline{U}_p^{m+1/2}) \nabla C^n, \nabla z) =$$

$$= (g(\check{C}^n), z) + ((\overline{U}_p^{m+1/2} - \overline{U}^n).\nabla \check{C}^n, z) +$$

$$+ ((D(\overline{U}_p^{m+1/2}) - D(\overline{U}^n)) \nabla \check{C}^n, \nabla z), \quad z \in M_h, \quad (2.19)$$

where the extrapolation $\check{C}^n$ is employed on the right-hand side so that linear algebraic equations with a constant matrix $\mathscr{C} + \Delta t_c \mathscr{A}(\overline{U}_p^{m+1/2})$ occur for t_c^m between t_p^m and t_p^{m+1}. The final algorithm consists of the combination of (2.8) at time t_p^m with (2.19) for $t_p^m < t_c^n \leqslant t_p^{m+1}$.

Variable time steps can be used in the following manner. The pressure steps can be changed arbitrarily without loss of algebraic efficiency. The integer Q occurring in the relation (2.7b) between Δt_p and Δt_c can be varied at each pressure step. But, Δt_c must be held fixed over any pressure step, for otherwise a new factorization would be required each time Δt_c changes and the efficiency of the method would evaporate.

The coefficients a_i, γ, and g are not necessarily defined for $c \notin [0, 1]$. Extend them continuously as constants in c on $(-\infty, 0] \cup [1, \infty)$, so that the numerical method, which does not preserve the maximum principle for the concentration that is satisfied for the differential problem, does not break down when C ranges outside $[0, 1]$.

3. SOME PRELIMINARIES FOR THE CONVERGENCE ANALYSIS

The analysis of the convergence of the scheme defined by (2.8) and (2.19) will be given under the assumption that the imposed flow is smoothly distributed. Thus, we shall be able to derive optimal order convergence results for smooth solutions. In the continuous-time case it was found valuable to introduce two projections in order to simplify the argument, and these projections are equally useful here. Let the pressure solution $\{ u, p \}$ be projected into the mixed finite element space by the map $\{ \tilde{U}, \tilde{P} \} : J \to V_h \times W_h$ given by

$$(a) \quad A(c; \tilde{U}, v) + B(v, \tilde{P}) = (\gamma(c), v), \quad v \in V_h,$$

$$(b) \quad B(\tilde{U}, \varphi) = -(q, \varphi), \quad \varphi \in W_h. \quad (3.1)$$

Then, by [4, (5.4)],

$$\| u - \tilde{U} \|_V + \| p - \tilde{P} \|_W \leqslant M \| p \|_{L^\infty (J; H^{k+3}(\Omega))} h_p^{k+1}, \quad t \in J. \quad (3.2)$$

Next, let $\tilde{C} : J \to M_h$ be the projection of c given by

$$(D(u) \nabla(\tilde{C} - c), \nabla z) + (u.\nabla(\tilde{C} - c), z) + (\lambda(\tilde{C} - c), z) = 0 , \quad z \in M_h ,$$

(3.3)

where

$$\lambda = 1 + q^+ .$$ (3.4)

Then, from [4, (5.10) and (5.11)],

(a) $\| c - \tilde{C} \|_{L^2(\Omega)} + h_c \| c - \tilde{C} \|_{H^1(\Omega)} \leqslant M_1 \| c \|_{H^{l+1}(\Omega)} h_c^{l+1} ,$

(3.5)

(b) $\left\| \dfrac{\partial(c - \tilde{C})}{\partial t} \right\|_{L^2(\Omega)} \leqslant M_2 \left\{ \| c \|_{H^{l+1}(\Omega)} + \left\| \dfrac{\partial c}{\partial t} \right\|_{H^{l+1}(\Omega)} \right\} h_c^{l+1} ,$

where both M_1 and M_2 depend on the L^∞-norm of u and the ellipticity constant associated with $d_m\phi(x)$ and M_2 depends on the L^∞-norm of $\partial u/\partial t$ as well.

The estimate [4, (6.2)] for $U - \tilde{U}$ and $P = \tilde{P}$ is valid at pressure time levels; thus,

$$\| U^m - \tilde{U}^m \|_V + \| P^m - \tilde{P}^m \|_W \leqslant M \| c(t_p^m) - C(t_p^m) \|_{L^2(\Omega)} . \quad (3.6)$$

The quasi-regularity of the grid has been assumed in the derivation of (3.6).

4. CONVERGENCE ANALYSIS

Let $\xi = C - \tilde{C}$ and $\eta = c - \tilde{C}$. Then, (2.4), (2.19), and (3.3) can be combined to obtain the relation

$$\left(\phi \frac{\xi^n - \xi^{n-1}}{\Delta t_c} , z \right) + (\overline{U}_p^{m+1/2}.\nabla\xi^n, z) + (D(\overline{U}_p^{m+1/2}) \nabla\xi^n, \nabla z) =$$

$$= \left(\phi \left\{ \frac{\tilde{C}^n - \tilde{C}^{n-1}}{\Delta t_c} - \frac{\partial c^n}{\partial t} \right\}, z \right) - (\lambda\eta^n, z) -$$
$$- ((\overline{U}_p^{m+1/2} - u^n).\nabla\tilde{C}^n, z) - ((D(\overline{U}_p^{m+1/2}) - D(u^n)) \nabla\tilde{C}^n, \nabla z)$$
$$+ (g(\check{C}^n) - g(c^n), z) + ((\overline{U}_p^{m+1/2} - \overline{U}^n).\nabla\tilde{C}^n, z)$$
$$+ ((D(\overline{U}_p^{m+1/2}) - D(\overline{U}^n)) \nabla\tilde{C}^n, \nabla z) , \quad z \in M_h . \quad (4.1)$$

The terms will be treated either separately or in combination below, and the test function will be chosen to be $z = \xi^n$.

First,

$$\frac{\tilde{C}^n - \tilde{C}^{n-1}}{\Delta t_c} - \frac{\partial c^n}{\partial t} = - \frac{1}{\Delta t_c} \int_{t_c^{n-1}}^{t_c^n} \frac{\partial\eta}{\partial t} d\tau - \frac{1}{\Delta t_c} \int_{t_c^{n-1}}^{t_c^n} (\tau - t_c^{n-1}) \frac{\partial^2 c}{\partial\tau^2} d\tau ,$$

and

$$\left| \left(\phi \left(\frac{\tilde{C}^n - \tilde{C}^{n-1}}{\Delta t_c} - \frac{\partial c^n}{\partial t} \right), \xi^n \right) \right| \leqslant M \left\{ (\Delta t_c)^{-1} \left\| \frac{\partial \eta}{\partial t} \right\|^2_{L^2(J^n; L^2)} + \right.$$

$$\left. + \Delta t_c \left\| \frac{\partial^2 c}{\partial t^2} \right\|^2_{L^2(J^n; L^2)} + \| \xi^n \|^2_{L^2} \right\} \quad (4.2)$$

where $J^n = (t_c^{n-1}, t_c^n)$ and the argument « Ω » will be omitted where the meaning is clear. Also,

$$| (\lambda \eta^n, \xi^n) | \leqslant M \{ \| \eta^n \|^2_{L^2} + \| \xi^n \|^2_{L^2} \} . \quad (4.3)$$

Next, note that

$$(D(u^n) - D(\overline{U}_p^{m+1/2})) \nabla \tilde{C}^n + (D(\overline{U}_p^{m+1/2}) - D(\overline{U}^n)) \nabla \check{C}^n =$$

$$= (D(\overline{U}^n) - D(\overline{U}_p^{m+1/2})) \nabla (\check{C}^n - 2 \tilde{C}^{n-1} + \tilde{C}^{n-2}) -$$

$$- (D(\overline{U}^n) - D(\overline{U}_p^{m+1/2})) \nabla (2 \xi^{n-1} - \xi^{n-2})$$

$$+ (D(u^n) - D(\overline{U}^n)) \nabla \tilde{C}^n \quad (4.4)$$

Observe that

$$\nabla (\tilde{C}^n - 2 \tilde{C}^{n-1} + \tilde{C}^{n-2}) = \Delta t_c \int_{t_c^{n-2}}^{t_c^n} \left(1 - \frac{| \tau - t_c^{n-1} |}{\Delta t_c} \right) \nabla \frac{\partial^2 \tilde{C}}{\partial t^2} d\tau .$$

Thus, using [4, (7.2)-(7.4)], we see that

$$| ((D(\overline{U}^n) - D(\overline{U}_p^{m+1/2})) \nabla (\tilde{C}^n - 2 \tilde{C}^{n-1} + \tilde{C}^{n-2}), \nabla \xi^n) | \leqslant$$

$$\leqslant M \| \overline{U}^n - \overline{U}_p^{m+1/2} \|_{L^2} \Delta t_c \left\| \int_{t_c^{n-2}}^{t_c^n} \left(1 - \frac{| \tau - t_c^{n-1} |}{\Delta t_c} \right) \nabla \frac{\partial^2 \tilde{C}}{\partial t^2} d\tau \right\|_{L^\infty} \| \nabla \xi^n \|_{L^2} .$$

Since

$$\overline{U}^n - \overline{U}_p^{m+1/2} = \frac{t_c^n - t_p^{m+1/2}}{\Delta t_p} (U^m - U^{m-1}),$$

it follows that $\| \overline{U}^n - \overline{U}_p^{m+1/2} \|_{L^2}$ is bounded. Indeed, by differencing the equations defining U^m and U^{m-1}, a factor of Δt_p should be obtainable through estimating $C(t_p^m) - C(t_p^{m-1})$; however, just boundedness suffices for our purposes. Thus,

$$| ((D(\overline{U}^n) - D(\overline{U}_p^{m+1/2})) \nabla (\tilde{C}^n - 2 \tilde{C}^{n-1} + \tilde{C}^{n-2}), \nabla \xi^n) | \leqslant$$

$$\leqslant \varepsilon \| \nabla \xi^n \|^2_{L^2} + M (\Delta t_c)^3 \left\| \frac{\partial^2 \tilde{C}}{\partial t^2} \right\|^2_{L^2(J^n \cup J^{n-1}; W^{1,\infty})} . \quad (4.5)$$

The term involving $\nabla(2\,\xi^{n-1} - \xi^{n-2})$ must be treated more carefully; here, it is necessary to see that $D(\overline{U}^n) - D(\overline{U}_p^{m+1/2})$ tends to zero as Δt_c tends to zero. We shall derive two estimates, one applicable to the case of the zero index Raviart-Thomas space and the other for positive index spaces. For the first of these estimates, we note that

(a) $\quad A(C(t_p^m); U^m - U^{m-1}, v) + B(v, P^m - P^{m-1}) =$

$$= \left(\left(\frac{1}{a(C(t_p^{m-1}))} - \frac{1}{a(C(t_p^m))}\right) U^{m-1}, v\right) + (\gamma(C(t_p^m)) - \gamma(C(t_p^{m-1})), v), \quad v \in V_h,$$

$$(4.6)$$

(b) $\quad B(U^m - U^{m-1}, \varphi) = (q(t_p^{m-1}) - q(t_p^m), \varphi), \quad \varphi \in W_h.$

Thus,

$$\| U^m - U^{m-1} \|_V + \| P^m - P^{m-1} \|_W \leqslant$$
$$\leqslant M \left\{ \Delta t_p + \| U^{m-1} \|_{L^\infty} \| C(t_p^m) - C(t_p^{m-1}) \|_{L^2} \right\} \quad (4.7)$$

and

$$\| \overline{U}^n - \overline{U}_p^{m+1/2} \|_V \leqslant M(p, c) \left\{ 1 + \left\| \frac{\xi_p^m - \xi_p^{m-1}}{\Delta t_p} \right\|_{L^2} \right\} \times$$
$$\times \left\{ 1 + h_p^{-1}(h_c^{l+1} + \| \xi_p^{m-1} \|_{L^2}) \right\} \Delta t_p, \quad (4.8)$$

where quasi-regularity has been invoked to shift $\| U^{m-1} \|_{L^\infty}$ to $\| U^{m-1} \|_{L^2}$ and then (3.6) and (3.5a) have been applied. The constant $M(p, c)$ depends on the $W^{1,\infty}$-norm of p^{m-1} and the H^{l+1}-norm of $c(t_p^{m-1})$. The notation ξ_p^m indicates $\xi(t_p^m)$. It then follows that

$$| ((D(\overline{U}^n) - D(\overline{U}_p^{m+1/2})) \nabla(2\,\xi^{n-1} - \xi^{n-2}), \nabla\xi^n) | \leqslant$$
$$\leqslant M(p, c) \left\{ 1 + \left\| \frac{\xi_p^m - \xi_p^{m-1}}{\Delta t_p} \right\|_{L^2} \right\} \left\{ 1 + h_p^{-1}(h_c^{l+1} + \| \xi_p^{m-1} \|_{L^2}) \right\} \frac{\Delta t_p}{h_c} \cdot$$
$$\cdot \left\{ \| \nabla\xi^n \|_{L^2}^2 + \| \nabla\xi^{n-1} \|_{L^2}^2 + \| \nabla\xi^{n-2} \|_{L^2}^2 \right\}, \quad (4.9)$$

where again an inverse property has been used to replace $\| \nabla\xi^n \|_{L^\infty}$ by $\| \nabla\xi^n \|_{L^2}$. The application of (4.9) will introduce a constraint of the form $\Delta t_p = o(h_c)$, which will not be serious for the choice $k = 0$ and $l = 1$ for the indices of the spaces but which is not natural for $k \geqslant 1$.

The second estimate for the $\nabla(2\,\xi^{n-1} - \xi^{n-2})$-term passes through an L^∞-estimate for $\overline{U}^n - \overline{U}_p^{m+1/2}$. First, write the difference in the form

$$\overline{U}^n - \overline{U}_p^{m+1/2} = (\overline{U}^n - \overline{u}^n) + (\overline{u}^n - \overline{u}_p^{m+1/2}) + (\overline{u}_p^{m+1/2} - \overline{U}_p^{m+1/2}). \quad (4.10)$$

Then,

$$\| \overline{U}^n - \overline{u}^n \|_{L^\infty} \leqslant 3 \{ \| U^m - u^m \|_{L^\infty} + \| U^{m-1} - u^{m-1} \|_{L^\infty} \}$$
$$\leqslant M(p, c) \{ h_p^k + h_p^{-1}(h_c^{l+1} + \| \xi_p^m \|_{L^2} + \| \xi_p^{m-1} \|_{L^2}) \}, \quad (4.11)$$

by (3.2), (3.5a), (3.6), and quasi-regularity; now, $M(p, c)$ depends on H^{k+3}-norms of p as well. The h_p^k-term should be improvable by the application of reasonable L^∞-estimates for $u - \tilde{U}$; Scholtz [14] has derived one for $k \geqslant 1$, but the case $k = 0$, which we would need to uniformize our argument, has not been treated. Then, (4.10), (4.11), and [4, (7.4)] imply that

$$| ((D(\overline{U}^n) - D(\overline{U}_p^{m+1/2})) \nabla(2 \xi^{n-1} - \xi^{n-2}), \nabla \xi^n) | \leqslant$$
$$\leqslant M(p, c) \{ h_p^k + h_p^{-1} h_c^{l+1} + h_p^{-1}(\| \xi_p^m \|_{L^2} + \| \xi_p^{m-1} \|_{L^2}) + \Delta t_p \} .$$
$$\cdot \{ \| \nabla \xi^n \|_{L^2}^2 + \| \nabla \xi^{n-1} \|_{L^2}^2 + \| \nabla \xi^{n-2} \|_{L^2}^2 \} . \quad (4.12)$$

Next, consider the final term generated by (4.4) :

$$| ((D(u^n) - D(\overline{U}^n)) \nabla \tilde{C}^n, \nabla \xi^n) | \leqslant$$
$$\leqslant | ((D(u^n) - D(\overline{u}^n)) \nabla \tilde{C}^n, \nabla \xi^n) | + | ((D(\overline{u}^n) - D(\overline{U}^n)) \nabla \tilde{C}^n, \nabla \xi^n) |$$
$$\leqslant M(p, c) \{ \| u^n - \overline{u}^n \|_{L^2} + \| \overline{u}^n - \overline{U}^n \|_{L^2} \} \| \nabla \xi^n \|_{L^2}$$
$$\leqslant M(p, c) \{ (\Delta t_p)^4 + h_p^{2k+2} + \| \xi_p^m \|_{L^2}^2 + \| \xi_p^{m-1} \|_{L^2}^2 \} + \varepsilon \| \nabla \xi^n \|_{L^2}^2 . \quad (4.13)$$

Three terms in (4.1) remain to be bounded. Again, two must be combined in like manner to that leading to (4.4) :

$$(u^n - \overline{U}^{m+1/2}).\nabla \tilde{C}^n + (\overline{U}^{m+1/2} - \overline{U}^n).\nabla \check{C}^n =$$
$$= (u^n - \overline{U}^n).\nabla \tilde{C}^n + (\overline{U}^n - \overline{U}^{m+1/2}).\nabla(\tilde{C}^n - 2 \tilde{C}^{n-1} + \tilde{C}^{n-2}) +$$
$$+ (\overline{U}_p^{m+1/2} - \overline{U}^n).\nabla(2 \xi^{n-1} - \xi^{n-2}) . \quad (4.14)$$

Now,

$$| ((u^n - \overline{U}^n).\nabla \tilde{C}^n, \xi^n) | \leqslant M(p, c) \{ (\Delta t_p)^2 + \| \overline{u}^n - \overline{U}^n \|_{L^2} \} \| \xi^n \|_{L^2}^2$$
$$\leqslant M(p, c) \{ (\Delta t_p)^4 + h_p^{2k+2} + \| \xi_p^m \|_{L^2}^2 +$$
$$+ \| \xi_p^{m-1} \|_{L^2}^2 + \| \xi^n \|_{L^2}^2 \} . \quad (4.15)$$

Next,

$$| ((\overline{U}^n - \overline{U}_p^{m+1/2}).\nabla(\tilde{C}^n - 2 \tilde{C}^{n-1} + \tilde{C}^{n-2}), \xi^n) | \leqslant M(p, c) \{ (\Delta t_p)^4 + \| \xi^n \|_{L^2}^2 \} .$$
$$(4.16)$$

In order to bound the third term arising from (4.14), recall [13] the embedding inequality for finite element spaces over quasi-regular polygonalizations given

by

$$\| \xi \|_{L^\infty} \leqslant M (\log h_c^{-1})^{1/2} (\| \nabla \xi \|_{L^2} + \| \xi \|_{L^2}), \qquad \xi \in M_h. \quad (4.17)$$

Then,

$$| ((\overline{U}_p^{m+1/2} - \overline{U}^n).\nabla(2 \xi^{n-1} - \xi^{n-2}), \xi^n) | \leqslant$$

$$\leqslant M \| \overline{U}_p^{m+1/2} - \overline{U}^n \|_{L^2} (\| \nabla \xi^{n-1} \|_{L^2} + \| \nabla \xi^{n-2} \|_{L^2}) \| \xi^n \|_{L^\infty}$$

$$\leqslant M(p, c) \{ h_p^{k+1} + h_c^{l+1} + \| \xi_p^m \|_{L^2} + \| \xi_p^{m-1} \|_{L^2} + \Delta t_p \}.$$

$$\cdot (\log h_c^{-1})^{1/2} \{ \| \xi^n \|_{L^2}^2 + \| \nabla \xi^n \|_{L^2}^2 + \| \nabla \xi^{n-1} \|_{L^2}^2 + \| \nabla \xi^{n-2} \|_{L^2}^2 \}. \quad (4.18)$$

The final term generated by (4.1) can be handled easily :

$$| (g(\check{C}^n) - g(c^n), \xi^n) | \leqslant | (g(\check{C}^n) - g(\check{c}^n), \xi^n) | + | (g(\check{c}^n) - g(c^n), \xi^n) | \leqslant$$

$$\leqslant M(p, c) \{ (\Delta t_c)^2 + h_c^{2l+2} + \| \xi^n \|_{L^2}^2 + \| \xi^{n-1} \|_{L^2}^2 + \| \xi^{n-2} \|_{L^2}^2 \}. \quad (4.19)$$

We turn now to estimating the left-hand side from below. It follows from Cauchy-Schwarz and [4, (5.9)] that

$$\left(\phi \frac{\xi^n - \xi^{n-1}}{\Delta t_c}, \xi^n \right) + (D(\overline{U}_p^{m+1/2}) \nabla \xi^n, \nabla \xi^n) \geqslant$$

$$\geqslant \frac{1}{2 \Delta t_c} \{ (\phi \xi^n, \xi^n) - (\phi \xi^{n-1}, \xi^{n-1}) \} + (\phi(d_m + d_t | U_p^{m+1/2} |) \nabla \xi^n, \nabla \xi^n).$$

$$(4.20)$$

The argument of [4, (7.8)-(7.9)] can be repeated with $\overrightarrow{U}_p^{m+1/2}$ in place of U to show that

$$| (\overline{U}_p^{m+1/2}.\nabla \xi^n, \xi^n) | \leqslant M(p, c) \{ 1 + \| \xi_p^m \|_{L^2}^2 + \| \xi_p^{m-1} \|_{L^2}^2 \} \| \xi^n \|_{L^2}^2 +$$

$$+ \varepsilon \| \nabla \xi^n \|_{L^2}^2. \quad (4.21)$$

The bounds derived above can be collected to imply the inequality (all norms are now in L^2 or $(L^2)^2$)

$$\frac{1}{\Delta t_c} \{ (\phi \xi^n, \xi^n) - (\phi \xi^{n-1}, \xi^{n-1}) \} + (\phi(d_m + d_t | \overline{U}_p^{m+1/2} |) \nabla \xi^n, \nabla \xi^n) \leqslant$$

$$\leqslant M(p, c) \{ h_c^{2l+2} + h_p^{2k+2} + (\Delta t_c)^2 + (\Delta t_p)^4 \} +$$

$$+ M(p, c) \{ 1 + \| \xi_p^m \|^2 + \| \xi_p^{m-1} \|^2 \} \{ \| \xi^n \|^2 + \| \xi^{n-1} \|^2 + \| \xi^{n-2} \|^2 \}$$

$$+ M(p, c) \{ \| \xi_p^m \|^2 + \| \xi_p^{m-1} \|^2 \} + Q^n + R_j^n \quad (4.22)$$

for $j = 1$ or 2, where

$$Q^n = M(p, c) (\log h_c^{-1})^{1/2} \{ h_p^{k+1} + h_c^{l+1} + \Delta t_p + \| \xi_p^m \| + \| \xi_p^{m-1} \| \}.$$
$$\cdot \{ \| \xi^n \|^2 + \| \nabla \xi^n \|^2 + \| \nabla \xi^{n-1} \|^2 + \| \nabla \xi^{n-2} \|^2 \} \quad (4.23)$$

and

(a) $R_1^n = M(p, c) \{ 1 + h_p^{-1} h_c^{l+1} + h_p^{-1} (\| \xi_p^m \| + \| \xi_p^{m-1} \|) \} \times$

$$\times \left\{ 1 + \left\| \frac{\xi_p^m - \xi_p^{m-1}}{\Delta t_p} \right\| \right\} \cdot \frac{\Delta t_p}{h_c} \{ \| \nabla \xi^n \|^2 + \| \nabla \xi^{n-1} \|^2 + \| \nabla \xi^{n-2} \|^2 \},$$

(b) $R_2^n = M(p, c) \{ h_p^k + \Delta t_p + h_p^{-1} h_c^{l+1} + h_p^{-1} (\| \xi_p^n \| + \| \xi_p^{m-1} \|) \}.$

$$\cdot \{ \| \nabla \xi^n \|^2 + \| \nabla \xi^{n-1} \|^2 + \| \nabla \xi^{n-2} \|^2 \}.$$

$$(4.24)$$

The $L^2(J^n; ...)$-terms have been replaced by $(\Delta t_c)^{1/2}$ times the corresponding $L^\infty(J^n; ...)$-terms on the right-hand side in (4.22) to simplify the appearance of the argument.

The object now is to demonstrate optimal order convergence in L^2 for the concentration; i.e., we wish to show that $\| \xi^n \| = 0(h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p)^2)$. In order to do so, certain constraints will be imposed on these four parameters; it will be shown later that the constraints are reasonable for the choices of the indices k and l that are likely to be used. The constraints will differ depending on whether R_1^n or R_2^n is chosen in the inequality (4.22). The demonstration also requires an induction argument, dependent again on the choice of R_1^n or R_2^n. For either choice, assume that

$$(\Delta t_p + h_p^{k+1}) (\log h_c^{-1})^{1/2} \to 0 \quad (4.25)$$

and make the induction hypothesis that

$$(\log h_c^{-1})^{1/2} \sup_n \| \xi^n \| \to 0. \quad (4.26)$$

These two hypotheses control the Q^n-terms, in that after summation in time, the H^1-portion of Q^n is covered asymptotically by a small fraction of the diffusion term on the left-hand side of (4.22).

To analyze (4.22) when R_1^n is to be considered, we require that

(a) $h_p^{-1}(h_c^{l+1} + \Delta t_c + (\Delta t_p)^2) \leqslant K_1$, a constant,

(b) $h_c^{-1}(\Delta t_p + h_p^{k+1}) \to 0.$

$$(4.27)$$

With these constraints, we make the induction hypothesis that

$$h_c^{-1} \sup_n \| \xi^n \| \to 0 . \tag{4.28}$$

When instead R_2^n is to be considered, we assume that

$$(a) \quad k \geqslant 1 , \quad \text{the Raviart-Thomas index} ,$$
$$(b) \quad h_p^{-1}(h_c^{l+1} + \Delta t_c + (\Delta t_p)^2) \to 0 , \tag{4.29}$$

and the required induction hypothesis is that

$$h_p^{-1} \sup_n \| \xi^n \| \to 0 . \tag{4.30}$$

Under either the conditions (4.27)-(4.28) or (4.29)-(4.30) in addition to (4.25)-(4.26), it follows that, as $(h, \Delta t) \to 0$,

$$\frac{1}{\Delta t_c} \{ (\phi \xi^n, \xi^n) - (\phi \xi^{n-1}, \xi^{n-1}) \} + (\phi (d_m + d_t | \overline{U}_p^{m+1/2} |) \nabla \xi^n, \nabla \xi^n) \leqslant$$

$$\leqslant M'(p, c) \{ h_c^{2l+2} + h_p^{2k+2} + (\Delta t_c)^2 + (\Delta t_p)^4 \} +$$

$$+ M''(p, c) \{ \| \xi^n \|^2 + \| \xi^{n-1} \|^2 + \| \xi^{n-2} \|^2 + \| \xi_p^m \|^2 + \| \xi_p^{m-1} \|^2 \}$$

$$+ \varepsilon \{ \| \nabla \xi^n \|^2 + \| \nabla \xi^{n-1} \|^2 + \| \nabla \xi^{n-2} \|^2 \} \tag{4.31}$$

for $t_p^m < t_c^n \leqslant t_p^{m+1}$ and $m \geqslant 1$. We remind the reader that this form is not quite appropriate for $t_c^n \leqslant t_p^1$, since the procedure has to be modified during the start-up process. We shall assume that the start-up procedure is such that

$$\sup_{0 \leqslant t_c^n \leqslant t_p^1} \{ \| \xi^n \| + \Delta t_c \| \nabla \xi^n \| \} \leqslant M(p, c) (h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p)^2) \} ;$$
$$\tag{4.32}$$

any reasonable scheme will suffice. Under this assumption we can consider $t_c^n > t_p^1$ and ignore the terms arising from times preceding t_p^1. Now, multiply (4.31) by Δt_c and add on the time for $t_p^1 < t_c^k \leqslant t_c^n$. Then, if

$$m(k) = m \qquad \text{for} \qquad t_p^m < t_c^k \leqslant t_p^{m+1} , \tag{4.33}$$

$$(\phi \xi^n, \xi^n) - (\phi \xi_p^1, \xi_p^1) + \sum_{t_p^1 < t_c^k \leqslant t_c^n} (\phi (d_m + d_t | \overline{U}_p^{m(k)+1/2} |) \nabla \xi^k, \nabla \xi^k) \Delta t_c \leqslant$$

$$\leqslant M' t_c^n \{ h_c^{2l+2} + h_p^{2k+2} + \Delta t_c + (\Delta t_p)^2 \} +$$

$$+ 3 M K'' \sum_{t_p^1 < t_c^k \leqslant t_c^n} (\| \xi^k \|^2 + \| \xi^{m(k)} \|^2) \Delta t_c$$

$$+ 3 \varepsilon \sum_{t_p^1 < t_c^k \leqslant t_c^n} \| \nabla \xi^k \|^2 \Delta t_c . \tag{4.34}$$

For ε sufficiently small the last term is covered by the diffusion term on the lefthand side, and it follows that

$$\| \xi^n \|^2 \leqslant M''' \{ h_c^{2l+2} + h_p^{2k+2} + (\Delta t_c)^2 + (\Delta t_p)^4 \} +$$

$$+ M''' \sum_{t_p^1 < t_c^k \leqslant t_c^n} (\| \xi^k \|^2 + \| \xi^{m(k)} \|^2) \Delta t_c . \quad (4.35)$$

Let

$$\alpha^n = \max \{ \| \xi^k \|^2 : t_p^1 < t_c^k \leqslant t_c^n \}, \quad (4.36)$$

so that

$$\alpha^n \leqslant M''' \{ h_c^{2l+2} + h_p^{2k+2} + (\Delta t_c)^2 + (\Delta t_p)^4) \} + 2 M''' \sum_{t_p^1 < t_c^k \leqslant t_c^n} \alpha^k \Delta t_c .$$

$$(4.37)$$

An application of the Gronwall lemma shows that

$$\| \xi^n \| \leqslant M(p, c) \{ h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p)^2 \}, \quad (4.38)$$

as was to have been shown. Thus, optimal order convergence will take place, provided that the induction hypotheses can be demonstrated. First, (4.26) follows from (4.25) and (4.38). Next, (4.28) follows from (4.27b), the fact that $\Delta t_c \leqslant \Delta t_p$, and (4.38). Finally, (4.30) follows from the two parts of (4.29) and (4.38). Hence, (4.38) is established.

If (4.38) is then combined with (3.5) and then with (3.2) and (3.6), we obtain the estimate

$$\max_n \| (c - C) (t_c^n) \|_{L^2} + \max_m [\| (u - U) (t_p^m) \|_V + \| (p - P) (t_p^m) \|_W] \leqslant$$

$$\leqslant M(p, c) \{ h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p)^2 \}, \quad (4.39)$$

where $M(p, c)$ depends on the norms of p in $L^\infty(J; W^{1,\infty})$ and $L^\infty(J; H^{k+3})$ and those of c in $H^2(J; W^{1,\infty})$ and $W^{1,\infty}(J; H^{l+1})$, provided that (4.25) and either (4.27) or (4.29) hold. The reasonableness of these restrictions will be discussed in the next section.

5. REASONABLENESS OF THE PARAMETER CONSTRAINTS

The most likely choices of the indices for the first element spaces are the pairs $(k, l) = (0, 1)$ and $(1, 1)$, and it is most important that the constraint (4.27) not be too restrictive for the $(0, 1)$-case and that (4.29) not be so for the $(1, 1)$-case. In fact, the only real restriction that is imposed for any choice (k, l) arises in the $(0, 1)$-case, and it is very slight. Since the error behaves asympto-

tically as

$$h_c^{l+1} + h_p^{k+1} + \Delta t_c + (\Delta t_p)^2 , \qquad (5.1)$$

the error is balanced by taking these four terms roughly equal in size. If this is done, then, for any $l \geqslant 1$,

$$h_p^{-1}(h_c^{l+1} + \Delta t_c + (\Delta t_p)^2) \sim h_p^k \to 0 \qquad (5.2)$$

if $k \geqslant 1$. Thus, (4.29) holds and the convergence rate is assured. If $k = 0$ and $l > 1$, then this choice of the parameters leads to

(a) $h_p^{-1}(h_c^{l+1} + \Delta t_c + (\Delta t_p)^2) \sim$ constant

(b) $h_c^{-1}(\Delta t_p + h_p) \sim h_c^{\frac{l-1}{2}} \to 0$,

and (4.27) holds, so that convergence is again assured at the optimal rate.

Finally, for the case $k = 0$ and $l = 1$, take $h_c^2 = \Delta t_c = (\Delta t_p)^2$ and $\Delta t_p = o(h_c)$. Again, (4.27) holds. We have had to choose the pressure step smaller than we should like, but not too seriously. Thus, in all cases very reasonable choices can be made for the parameters h_c, h_p, Δt_c and Δt_p.

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