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AN ALTERNATING DIRECTION GALERKIN METHOD COMBINED WITH A MODIFIED METHOD OF CHARACTERISTICS FOR MISCIBLE DISPLACEMENT INFLUENCED BY MOBILE AND IMMOBILE WATER

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Abstract. Numerical approximations are considered for a mathematical model for miscible displacement influenced by mobile and immobile water. A mixed finite element method is adopted to give a direct approximation of the velocity, the concentration in mobile water is approximated by an alternating direction Galerkin finite element method combined with the method of characteristics and the concentration in immobile water is approximated by a standard Galerkin method. Optimal order L^2- and H^1-error estimates are derived.

Key Words. alternating direction Galerkin method, modified method of characteristic, finite element methods, error estimate.

1. Introduction

In recent years, the intentional or accidental release of chemical wastes on soils has further stimulated current interests in the movement of chemicals. Displacement studies have become important tools in soil physics, particularly for predicting the movement of pesticide, nitrates, heavy metals, and other solutes through soils.

The soil structure is complex. In aggregated media, soils are composed of slowly and quickly conducting pore sequences, the liquid-filled and dead-end pores; or immobile water exists. In [12] the movement of a chemical through a sorbing porous medium with a lateral or intra-aggregated diffusion was considered. The liquid in porous media is divided into mobile and immobile regions. Mobile water is located inside the larger pores. The flow in mobile water is assumed to occur in this region only. Solute transfer in mobile water occurs by both convection and longitudinal diffusion. Immobile water is located inside aggregates and at the contact points of aggregates and/or particles. Diffusion transfer between the two liquid regions is assumed to be proportional to the concentration difference between the mobile and immobile liquids. A dynamic soil region is located sufficiently close to the mobile water phase for equilibrium between the solute in the mobile liquid and that sorbed by this part of the soil mass. A stagnant soil region, where sorption is diffusion limited, is located mainly around the micro-pores inside the aggregates or along dead-end water pockets. Sorption occurs here only after the chemicals have diffused through the liquid barrier of the immobile liquid phase. In [12] sorption

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process in both the dynamic and stagnant regions of the medium was assumed to be instantaneous and the adsorption isotherm was assumed to be linear.

The Darcy velocity of the fluid mixture is given by [2, 3, 4]

$$\mathbf{u} = -a(c)\nabla p \;, \tag{1.1}$$

where $a(c) = \kappa(x)/\nu(c)$, κ is the permeability of the medium, ν the concentration-dependent viscosity, and p the pressure. Incompressibility implies

$$\nabla \cdot \mathbf{u} = q, \tag{1.2}$$

where $q = q(x,t)$ is the imposed external flow. The equation for the concentration can be put in the form [2, 12, 14]:

$$s_1\frac{\partial c}{\partial t} + s_2\frac{\partial c'}{\partial t} + \mathbf{u}\cdot\nabla c - \nabla\cdot(D\nabla c) = q(c^* - c), \quad x \in \Omega, \quad t \in J, \tag{1.3}$$

$$\frac{\partial c'}{\partial t} = \alpha(c - c'), \quad x \in \Omega, \quad t \in J, \tag{1.4}$$

where $J = [0,T]$, $s_1(x) = (\theta_m + f\rho K)/\theta_m, s_2(x) = (\theta_{im} + (1-f)\rho K)/\theta_{im}$, and $\alpha = \alpha_0/(\theta_{im} + (1-f)\rho K)$; f is the fraction adsorption in dynamic region; K the constant in the Freundlich isotherm; θ_m and θ_{im} the mobile water and immobile water content, respectively; ρ the bulk density; c and c' denote the solute concentrations in the mobile water and immobile water regions, respectively; D the dispersion coefficient, α_0 the mass exchange coefficient; c^* the concentration of the contamination.

The boundary and initial conditions can be imposed in the following form:

$$\mathbf{u}\cdot\mathbf{n} = 0, \quad D\nabla c\cdot\mathbf{n} = 0, \quad x \in \partial\Omega, \quad t \in J, \tag{1.5}$$

$$c(x,0) = c_0(x), \quad c'(x,0) = c_0'(x), \quad x \in \Omega, \tag{1.6}$$

where $\mathbf{n}$ is the unit outward normal to the boundary $\partial\Omega$ of the domain Ω. For compatibility one requires that

$$\int_\Omega q(x,t)dx = 0, \qquad \text{for all } \ t \in J.$$

Our objective is to design and analyze a numerical method for approximating the solution of the system (1.1)–(1.4) subject to the initial and boundary conditions (1.5) and (1.6). Note that the pressure does not appear explicitly in the equation (1.3) for concentration; however, velocity does. A mixed finite element method will be adopted here to approximate the pressure p and the velocity $\mathbf{u}$ simultaneously. The concentration c' in the immobile water will be approximated using a standard Galerkin finite element method. The concentration c in the mobile water will be approximated by an alternating direction method combined with the method of characteristics which combines the attractive attributes of the two methods.

In 1971, Douglas and Dupont in [9] formulated a Galerkin alternating-direction procedures for nonlinear parabolic equations posed on a rectangular region with a uniform grid. The alternating-direction method reduces multidimensional problems to a collection of one-dimensional problems and the matrices that must be inverted at each time step of the solution process are independent of time and require only one decomposition. The storage requirements for these matrices are associated with one-dimensional problems rather than the full multi-dimensional problem, so the storage requirements can be quite low. The Galerkin alternating-direction method is particularly attractive for solving large three-dimensional nonlinear problems. A survey of some results in the use of the alternating-direction finite element methods for linear and nonlinear partial differential equations was presented by Ewing [11]. Dendy and Fairweather [6] extended these methods on rectangles to certain unions of rectangles. Hayes [10] further generalized these methods to non-rectangular regions that can be isoparametrically mapped onto a rectangle.

The modified method of characteristics is attractive for convection-diffusion problems, which reflects the physical characters more clearly, produces much smaller time truncation error, and therefore allows for larger time steps than those of the standard methods.

For the sake of simplicity, we assume $\Omega = [0,1]^3$ is the unit cube and the coefficients a, s_1, s_2 and D are bounded both above and blow by positive constants:

$$0 < a_* \le a(c) \le a^*, \quad 0 < D_* \le D \le D^*,$$

$$0 < s_{1*} \le s_1(x) \le s_1^*, \quad 0 < s_{2*} \le s_2(x) \le s_2^*,$$

where $a_*, a^*, s_{1*}, s_1^*, s_{2*}, s_2^*, D_*$, and D^* are positive constants.

Throughout the paper, M stands for a general positive constant and has different meanings in different places.

The organization of the paper is as follows. In Section 2, a weak form of the problem is presented and the approximation procedure based on an alternating-direction Galerkin method combined with a modified method of characteristics is formulated. The convergence analysis is given in Section 3, where a-priori error estimates in both L^2- and H^1- norms are derived.

2. The Approximation Procedure

We will use the standard notation for the Sobolev spaces $H^m(\Omega)$ and $L^2(\Omega)$ and their corresponding norms $\|\cdot\|_m$ and $\|\cdot\|$. The inner product in $L^2(\Omega)$ is denoted by

$$(f,g) = \int_\Omega fg dx.$$

We also define the following vector-valued function space:

$$H(\mathrm{div};\Omega) = \{\mathbf{v}: \ \mathbf{v} \in L^2(\Omega)^3, \ \nabla\cdot\mathbf{v} \in L^2(\Omega)\}$$

equipped with the norm

$$\|\mathbf{v}\|_{H(\mathrm{div};\Omega)} = \left(\|\mathbf{v}\|^2 + \|\nabla\cdot\mathbf{v}\|^2\right)^{1/2}$$

and let

$$\mathbf{V} = \{\mathbf{v} \in H(\mathrm{div};\Omega): \ \mathbf{v}\cdot\mathbf{n} = 0 \text{ on } \partial\Omega\}$$

and

$$W = L^2(\Omega)/\left\{\varphi: \ \varphi \text{ is contant on } \Omega\right\}.$$

The finite element discretization of the problem (1.1)–(1.4) is based on the following weak formulation: Find $\{u,p,c,c'\} \in V\times W\times H^1(\Omega)\times L^2(\Omega)$ such that:

$$(a(c)^{-1}\mathbf{u}, v) - (\nabla\cdot v, p) = 0, \quad \forall\, v \in V, \tag{2.1}$$

$$(\nabla\cdot\mathbf{u}, \varphi) = (q,\varphi), \qquad \forall\, \varphi \in W, \tag{2.2}$$

$$\begin{aligned} &\left(s_1\frac{\partial c}{\partial t}, z\right) + \left(s_2\frac{\partial c'}{\partial t}, z\right) + (\mathbf{u}\cdot\nabla c, z) + (D\nabla c, \nabla z) \\ &= \quad (q(c^*-c), z), \quad \forall\, z \in H^1(\Omega), \ 0 < t \le T, \end{aligned} \tag{2.3}$$

$$\left(\frac{\partial c'}{\partial t}, z'\right) = (\alpha(c-c'), z'), \quad \forall\, z' \in L^2(\Omega), \ 0 < t \le T, \tag{2.4}$$

and $c(x,0) = c_0(x)$ and $c'(x,0) = c'_0(x)$.

Let $\mathcal{J}_{h_c}$, $\mathcal{J}_{h_{c'}}$ and $\mathcal{J}_{h_p}$ denote three rectangular partitions of Ω with their respective mesh sizes h_c, $h_{c'}$, and h_p. To discretize equations (2.1), (2.2), (2.3) and (2.4), we introduce the following finite element spaces:

$$M_h = \{z \in H^1(\Omega) : \ z|_e \in \mathcal{Q}_\ell \text{ for any } e \in \mathcal{J}_{h_c}\},$$
$$N_h = \{z' \in L^2(\Omega) : \ z'|_e \in \mathcal{Q}_r \text{ for any } e \in \mathcal{J}_{h_{c'}}\},$$
$$\mathbf{V}_h = \tilde{\mathbf{V}}_h \cap \mathbf{V}, \quad W_h = \tilde{W}_h / \{\varphi : \ \varphi \text{ is constant on } \Omega\}.$$

Here $\mathcal{Q}_m$ ($m > 0$) is the set of all polynomials whose degree in each variable is no more than m, and $(\tilde{\mathbf{V}}_h, \tilde{W}_h)$ denotes the pair of the Raviart-Thomas spaces of order $k \geq 0$ defined on the mesh $\mathcal{J}_{h_p}$ [1, 7, 8, 15].

We now collect the following well-known approximation properties for the spaces M_h, N_h, $\mathbf{V}_h$ and W_h.

$$\inf_{z_h \in M_h} \|z - z_h\|_j \leq M\|z\|_{\ell+1} h_c^{\ell+1-j} \ , \ \forall \ \ z \in H^{\ell+1}(\Omega) \text{ and } j = 0, 1, \tag{2.5}$$

$$\inf_{z'_h \in N_h} \|z' - z'_h\| \leq M\|z'\|_{r+1} h_{c'}^{r+1} \ , \ \forall \ z' \in H^{1+r}(\Omega), \tag{2.6}$$

$$\inf_{\mathbf{v}_h \in \mathbf{V}_h} \|\mathbf{v} - \mathbf{v}_h\|_{L^2(\Omega)^3} \leq M\|\mathbf{v}\|_{H^{k+1}(\Omega)^3} h_p^{k+1} \ , \ \forall \ \mathbf{v} \in \mathbf{V}, \tag{2.7}$$

$$\inf_{\mathbf{v}_h \in \mathbf{V}_h} \|\mathbf{v} - \mathbf{v}_h\|_{H(\mathrm{div};\Omega)} \leq M\{\|\mathbf{v}\|_{H^{k+1}(\Omega)^3} + \|\nabla \cdot \mathbf{v}\|_{H^{k+1}(\Omega)}\} h_p^{k+1} \ , \ \forall \ \mathbf{v} \in \mathbf{V}, \tag{2.8}$$

$$\inf_{w_h \in W_h} \|w - w_h\|_W \leq M\|w\|_{H^{k+1}(\Omega)} h_p^{k+1}, \ \forall \ w \in W. \tag{2.9}$$

By a standard inverse property and the approximation property (2.5), we have

$$\inf_{z \in M_h} \sum_{e \in \mathcal{J}_{h_c}} \left\| \frac{\partial^m (u - z)}{\partial x_1^{m_1} \partial x_2^{m_2} \partial x_3^{m_3}} \right\|_{L^2(e)} \leq M\|u\|_{\ell+1} h_c^{\ell+1-m} \tag{2.10}$$

for $m = m_1 + m_2 + m_3$, $m_1 \geq 0$, $m_2 \geq 0$ and $m_3 \geq 0$.

In order to define the alternating-direction Galerkin method, we write

$$M_h = M_h^{x_1} \otimes M_h^{x_2} \otimes M_h^{x_3},$$

where $\otimes$ denotes the tensor product. Let $\{\Phi^1_\alpha(x_1)\}_{\alpha=1}^{N_1}$, $\{\Phi^2_\beta(x_2)\}_{\beta=1}^{N_2}$, $\{\Phi^3_\gamma(x_3)\}_{\gamma=1}^{N_3}$ be the bases for $M_h^{x_1}$, $M_h^{x_2}$ and $M_h^{x_3}$, respectively. Then any $C \in M_h$ can be written as

$$C = \sum_{\alpha=1}^{N_1} \sum_{\beta=1}^{N_2} \sum_{\gamma=1}^{N_3} C_{\alpha,\beta,\gamma} \Phi^1_\alpha(x_1) \Phi^2_\beta(x_2) \Phi^3_\gamma(x_3). \tag{2.11}$$

For any continuous function $s(x)$, its patch approximation $\bar{s}$ is defined as follows: If Ψ_j ($j = 1, \cdots, N_1N_2N_3$) are the bases of M_h and $e_{ij} = \mathrm{supp}(\Psi_i) \cap \mathrm{supp}(\Psi_j)$, we define $\bar{s} = \sqrt{s(x^i)} \cdot \sqrt{s(x^j)}$ on e_{ij}, where $x^i \in \mathrm{supp}(\Psi_i)$. In practice, x^i is chosen to be the node point associated with the basis function Ψ_i. It can be shown that for such a choice of $\bar{s}$ and for sufficiently small h we have

$$\sup_{x \in \Omega_i} |\bar{s}_1(x^i) - s_1(x^i)| = o(1). \tag{2.12}$$

For the time discretization, we partition the time interval $[0, T]$ into the following time steps:

$$0 = t^0 < t^1 < \cdots < t^N = T$$

with $\Delta t = T/N$ and $t^i = t^{i-1} + \Delta t$ ($i = 1, \cdots, N$).

The modified method of characteristics is a time-stepping procedure that can be combined with any spatial discretization. To apply this method to our problem, let τ denote the unit vector in the characteristic direction and $\psi = (s_1^2 + |\mathbf{u}|^2)^{1/2}$; then it follows

$$\psi \frac{\partial c}{\partial \tau} = s_1 \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c,$$

and (2.3) becomes:

$$\left(\psi \frac{\partial c}{\partial \tau}, z\right) + \left(s_2 \frac{\partial c'}{\partial t}, z\right) + (D\nabla c, \nabla z) = (q(c^* - c), z), \quad \forall\ z \in H^1(\Omega). \tag{2.13}$$

For a function $\varphi = \varphi(x,t)$, let $\varphi^n = \varphi(x, t^n)$. We approximate the directional derivative $\frac{\partial c^{n+1}}{\partial \tau}(x) = \frac{\partial c}{\partial \tau}(x, t^{n+1})$ by a backward difference quotient in the $\tau-$direction:

$$\frac{\partial c^{n+1}}{\partial \tau}(x) \approx \frac{s_1}{\psi} \frac{c^{n+1}(x) - \hat{c}^n(x)}{\Delta t}$$

where

$$\hat{c}^n(x) = c^n(\hat{x}),\ \hat{x} = x - \frac{\mathbf{u}^n(x)}{s_1(x)} \Delta t.$$

For (1.3)–(1.6) the characteristic–alternating direction finite element schemes are: assuming $\{\mathbf{u}_h^n, p_h^n, C^n, C'^n\}$ are known, find $\{\mathbf{u}_h^{n+1}, p_h^{n+1}, C^{n+1}, C'^{n+1}\} \in V_h \times W_h \times M_h \times N_h$ such that:

$$\begin{aligned}
&\left(\bar{s}_1 \frac{C^{n+1} - C^n}{\Delta t}, z\right) + (s_2 \frac{C'^{n+1} - C'^n}{\Delta t}, z) \\
&\quad + \lambda \left(\bar{s}_1 \nabla (C^{n+1} - C^n), \nabla z\right) \\
&\quad + \lambda^2 \Delta t \sum_{i \neq j, i,j=1}^{3} \left(\bar{s}_1 \frac{\partial^2 (C^{n+1} - C^n)}{\partial x_i \partial x_j}, \frac{\partial^2 z}{\partial x_i \partial x_j}\right) \\
&\quad + \lambda^3 \Delta t^2 \left(\bar{s}_1 \frac{\partial^3 (C^{n+1} - C^n)}{\partial x_1 \partial x_2 \partial x_3}, \frac{\partial^3 z}{\partial x_1 \partial x_2 \partial x_3}\right) \\
&= (q(C^{*n} - C^n), z) + ((\bar{s}_1 - s_1) \frac{C^n - C^{n-1}}{\Delta t}, z) \\
&\quad - (D\nabla C^n, \nabla z) - (s_1 \frac{C^n - \hat{C}^n}{\triangle t}, z),\ \forall\ z \in M_h,
\end{aligned} \tag{2.14}$$

$$\left(\frac{C'^{n+1} - C'^n}{\Delta t}, z'\right) = (\alpha(C^n - C'^{n+1}), z'),\ \forall\ z' \in N_h, \tag{2.15}$$

$$(a(C^{n+1})^{-1} \mathbf{u}_h^{n+1}, \mathbf{v}) - (\nabla \cdot \mathbf{v}, p_h^{n+1}) = 0,\ \forall\ \mathbf{v} \in \mathbf{V}_h, \tag{2.16}$$

$$(\nabla \cdot \mathbf{u}_h^{n+1}, \varphi) = (q, \varphi),\ \forall\ \varphi \in W_h. \tag{2.17}$$

Here the initial values $C(0) \in M_h$ and $C'(0) \in N_h$ are chosen as approximations of $c_0(x)$ and $c_0'(x)$, respectively; λ is a constant such that $\lambda > \frac{1}{2} \frac{D^*}{s_{1*}}$; $\bar{s}_1$ is the patch approximation of $s_1(x)$.

According to the structure of the basis functions in M_h, the approximation C of the concentration has a representation (2.11) in terms of the one-dimensional basis functions in each axis direction. We have the following equation:

$$(D^n)^{\frac{1}{2}}(B^{x_1} + \lambda\Delta t A^{x_1}) \otimes (B^{x_2} + \lambda\Delta t A^{x_2}) \otimes(B^{x_3} + \lambda\Delta t A^{x_3})(D^n)^{\frac{1}{2}}(C^{n+1} - C^n) = \Delta t F^n, \tag{2.18}$$

where B^{x_1}, A^{x_1}, B^{x_2}, A^{x_2}, B^{x_3} and A^{x_3} are matrices whose entries are given by

$$B^{x_1}_{\alpha_1,\alpha_2} = \int_0^1 \Phi^1_{\alpha_1}\Phi^1_{\alpha_2}dx_1, \quad A^{x_1}_{\alpha_1,\alpha_2} = \int_0^1 \frac{d\Phi^1_{\alpha_1}}{dx_1}\frac{d\Phi^1_{\alpha_2}}{dx_1}dx_1,$$
$$B^{x_2}_{\beta_1,\beta_2} = \int_0^1 \Phi^2_{\beta_1}\Phi^2_{\beta_2}dx_2, \quad A^{x_2}_{\beta_1,\beta_2} = \int_0^1 \frac{d\Phi^2_{\beta_1}}{dx_2}\frac{\Phi^2_{\beta_2}}{dx_2}dx_2,$$
$$B^{x_3}_{\gamma_1,\gamma_2} = \int_0^1 \Phi^3_{\gamma_1}\Phi^3_{\gamma_2}dx_3, \quad A^{x_3}_{\gamma_1,\gamma_2} = \int_0^1 \frac{d\Phi^3_{\gamma_1}}{dx_3}\frac{d\Phi^3_{\gamma_2}}{dx_3}dx_3,$$

D^n is the diagonal matrix

$$D^n = \mathrm{diag}\left(\bar{s}_1(x^1), \bar{s}_1(x^2)\cdots, \bar{s}_1(x^M)\right), \ M = N_1N_2N_3,$$

and F^n is the vector

$$F^n = (F^n_{\alpha,\beta,\gamma}, \alpha = 1,\cdots, N_1, \beta = 1,\cdots, N_2, \gamma = 1, \cdots, N_3)$$

with

$$\begin{aligned} F^n_{\alpha,\beta,\gamma} &= -(D\nabla C^n, \nabla(\Phi^1_\alpha \otimes \Phi^2_\beta \otimes \Phi^3_\gamma)) \\ &\quad -((s_1 - \bar{s}_1)\frac{C^n - C^{n-1}}{\Delta t}, \Phi^1_\alpha \otimes \Phi^2_\beta \otimes \Phi^3_\gamma) - \left(s_1\frac{C^n - \bar{C}^n}{\Delta t}, \Phi^1_\alpha \otimes \Phi^2_\beta \otimes \Phi^3_\gamma\right) \\ &\quad -(s_2\frac{{C'}^{n+1} - {C'}^n}{\Delta t}, \Phi^1_\alpha \otimes \Phi^2_\beta \otimes \Phi^3_\gamma) + (q(C^{*n} - C^n), \Phi^1_\alpha \otimes \Phi^2_\beta \otimes \Phi^3_\gamma). \end{aligned}$$

We point out that (2.18) can be solved by the alternating-direction Galerkin method.

3. Convergence analysis

In this section, we prove error estimates for the finite element approximations introduced in the previous section. Before we state our results, we introduce some notation. For each $t \in [0, T]$, let $(\tilde{\mathbf{u}}, \tilde{p}, \tilde{c}, \tilde{c'}) \in \mathbf{V}_h \times W_h \times M_h \times N_h$ be a projection of $(\mathbf{u}, p, c, c')$ defined through the following equations:

$$(a(c)^{-1}\tilde{\mathbf{u}}, \mathbf{v}) - (\nabla\cdot\mathbf{v}, \tilde{p}) = 0, \ \forall\ \mathbf{v} \in \mathbf{V}_h, \tag{3.1}$$

$$(\nabla\cdot\tilde{\mathbf{u}}, \varphi) = (q, \varphi), \ \forall\ \varphi \in W_h, \tag{3.2}$$

$$(D\nabla(\tilde{c} - c), \nabla z) + (\mu(\tilde{c} - c), z) = 0, \ \forall\ z \in M_h, \tag{3.3}$$

$$(\tilde{c'}, z') = (c', z'), \quad \forall\ z' \in N_h. \tag{3.4}$$

The function $\mu > 0$ in (3.3) is to assure the coercivity of the form.

In view of (2.1), (2.2), (3.1) and (3.2), $(\tilde{\mathbf{u}}, \tilde{p})$ is the mixed finite element approximation of $(\mathbf{u}, p)$. According to the well-known error estimates for the mixed finite element method [7], we have

$$\|\mathbf{u} - \tilde{\mathbf{u}}\|_{H(\mathrm{div};\Omega)} + \|p - \tilde{p}\|_W \le M\|p\|_{k+3}h_p^{k+1}. \tag{3.5}$$

Since $\tilde{c}$ is the Galerkin projection of c and $\tilde{c'}$ is the L^2 projection of c', we have the following error estimates [1, 16]:

$$\|c - \tilde{c}\| + h_c\|c - \tilde{c}\|_1 \le M\|c\|_{l+1}h_c^{l+1}, \tag{3.6}$$

$$\left\|\frac{\partial}{\partial t}(c-\tilde{c})\right\| \leq M\left\{\|c\|_{l+1}+\left\|\frac{\partial c}{\partial t}\right\|_{l+1}\right\} h_c^{l+1}, \tag{3.7}$$

$$\|c'-\tilde{c'}\| \leq M\|c'\|_{r+1} h_{c'}^{r+1}, \tag{3.8}$$

$$\left\|\frac{\partial}{\partial t}(c'-\tilde{c'})\right\| \leq M\left\|\frac{\partial c'}{\partial t}\right\|_{r+1} h_{c'}^{r+1}. \tag{3.9}$$

We split the errors into two terms:

$$C-c=\xi-\eta, \quad C'-c'=\rho-\zeta,$$

where

$$\xi=C-\tilde{c}, \quad \eta=c-\tilde{c},$$
$$\rho=C'-\tilde{c'}, \quad \zeta=c'-\tilde{c'}.$$

Our main results are stated in the following theorem.

Theorem 3.1. *Suppose that the exact solution of problem (1.3) and (1.4) is sufficiently smooth and the time and space discretization are such that*

$$\Delta t=O(h_p^2), \quad h_p^{-\frac{3}{2}}(h_c^{l+1}+h_c'^{r+1}) \to 0, \quad \text{as} \quad h \to 0, \tag{3.10}$$

and $\Delta t=O(h_c^2)$ *and* $\lambda>\frac{D^*}{2s_{1*}}$, $k \geq 1, l \geq 1$. *If the initial approximations satisfy*

$$\begin{aligned} &\|\rho^0\|^2+\|\rho^1\|^2+\|\xi^0\|_1^2+\|\xi^1\|_1^2+\Delta t\|d_t\xi^0\|^2 \\ \leq &M\{(\Delta t)^2+h_p^{2k+2}+h_c^{2l+2}+h_c'^{2r+2}\}, \end{aligned} \tag{3.11}$$

then the following error estimate holds:

$$\begin{aligned} &\max_n\{\|c'^n-C'^n\|^2+\|c^n-C^n\|^2+h_c\|c^n-C^n\|_1^2 \\ &+\sum_{k=0}^{n}\|d_t(c^k-C^k)\|^2\Delta t+\|p_h^n-p_h^n\|_W^2+\|\mathbf{u}^n-\mathbf{u}_h^n\|_V^2\} \\ &\leq M\{h_c^{2l+2}+h_{c'}^{2r+2}+h_p^{2k+2}+(\Delta t)^2\}, \end{aligned} \tag{3.12}$$

where $M>0$ *is a constant independent of* $h_p, h_c, h_{c'}$ *and* Δt

Proof. From (2.1), (2.2), (2.16) and (2.17), as well as the definitions of $\tilde{\mathbf{u}}$ and $\tilde{p}$, we have

$$\begin{aligned} &(a(C^{n+1})^{-1}(\mathbf{u}_h^{n+1}-\tilde{\mathbf{u}}^{n+1}),\mathbf{v})-(\nabla\cdot\mathbf{v},p_h^{n+1}-\tilde{p}^{n+1}) \\ &\quad= \quad (a(c^{n+1})^{-1}\tilde{\mathbf{u}}^{n+1},\mathbf{v})-(a(C^{n+1})^{-1}\tilde{\mathbf{u}}^{n+1},\mathbf{v}), \qquad \mathbf{v}\in\mathbf{V}_h, \end{aligned} \tag{3.13}$$

and

$$(\nabla\cdot(\mathbf{u}_h^{n+1}-\tilde{\mathbf{u}}^{n+1}),\varphi)=0, \qquad \varphi\in W_h. \tag{3.14}$$

From [8] we obtain:

$$\|\mathbf{u}_h^{n+1}-\tilde{\mathbf{u}}^{n+1}\|_{H(\mathrm{div};\Omega)}+\|p_h^{n+1}-\tilde{p}^{n+1}\|_W \leq M\|c^{n+1}-C^{n+1}\|. \tag{3.15}$$

Combining (2.4), (2.15) and (3.4) leads to the following error equation for c' and C':

$$(d_t\rho^n,z')=(\alpha(\xi^n-\eta^n)-\alpha(\rho^{n+1}-\zeta^{n+1}),z')+\left(\frac{\partial c'^{n+1}}{\partial t}-\frac{c'^{n+1}-c'^n}{\Delta t},z'\right). \tag{3.16}$$

Choosing $z'=\rho^n$ and then $z'=d_t\rho^n$ in (3.16), we obtain

$$\frac{1}{\Delta t}(\|\rho^{n+1}\|^2-\|\rho^n\|^2) \leq M\left\{\|\xi^n\|^2+\|\rho^{n+1}\|^2+h_c^{2l+2}+h_{c'}^{2r+2}+(\Delta t)^2\right\} \tag{3.17}$$

and

$$\|d_t\rho^n\|^2 \le M\left\{\|\xi^n\|^2+\|\rho^{n+1}\|^2+h_c^{2l+2}+h_{c'}^{2r+2}+(\Delta t)^2\right\}. \tag{3.18}$$

Next, we turn to the error equation for c and C. In fact, by a simple manipulation, the equations (2.3), (2.14) and (3.4) imply

$$\begin{aligned}
&(s_1 d_t\xi^n, z) + ((\bar{s}_1 - s_1)(d_t\xi^n - d_t\xi^{n-1}), z) + (D\nabla\xi^n, \nabla z)\\
&\quad +\lambda\Delta t\,(s_1\nabla d_t\xi^n,\nabla z) + (\lambda\Delta t)^2\sum_{i\neq j,i,j=1}^{3}\left(\bar{s}_1\frac{\partial^2 d_t\xi^n}{\partial x_i\partial x_j},\frac{\partial^2 z}{\partial x_i\partial x_j}\right)\\
&\quad +(\lambda\Delta t)^3\left(s_1^n\frac{\partial^3 d_t\xi^n}{\partial x_1\partial x_2\partial x_3},\frac{\partial^3 z}{\partial x_1\partial x_2\partial x_3}\right)\\
=&\quad \lambda\triangle t((s_1-\bar{s}_1)\nabla d_t\xi^n,\nabla z) + ((s_1^n-\bar{s}_1^n)(d_t\tilde{c}^n - d_t\tilde{c}^{n-1}), z)\\
&\quad -\lambda\Delta t\,(\bar{s}_1\nabla d_t\tilde{c}^n,\nabla z) + \left(s_1\frac{\partial c^{n+1}}{\partial t} + \mathbf{u}_h^n\cdot\nabla c^{n+1} - s_1\frac{c^{n+1}-\bar{c}^n}{\Delta t}, z\right)\\
&\quad +\left(s_1\frac{\bar{\xi}^n-\xi^n}{\Delta t}, z\right) + \left(s_1\frac{\eta^{n+1}-\bar{\eta}^n}{\Delta t}, z\right)\\
&\quad +\left(s_2\left(\frac{\partial c'^{n+1}}{\partial t} - \frac{C'^{n+1}-C'^n}{\Delta t}\right), z\right) - \mu(\eta^n, z)\\
&\quad +((\mathbf{u}^{n+1}-\mathbf{u}_h^n)\cdot\nabla c^n, z) - (\lambda\Delta t)^2\sum_{i\neq j,i,j=1}^{3}\left(\bar{s}_1\frac{\partial^2 d_t\tilde{c}^n}{\partial x_i\partial x_j},\frac{\partial^2 z}{\partial x_i\partial x_j}\right)\\
&\quad -(\lambda\Delta t)^3\left(\bar{s}_1\frac{\partial^3 d_t\tilde{c}^n}{\partial x_1\partial x_2\partial x_3},\frac{\partial^3 z}{\partial x_1\partial x_2\partial x_3}\right)\\
&\quad +(q(C^{*n}-C^n) - q(c^{*n+1}-c^{n+1}), z).
\end{aligned} \tag{3.19}$$

We now take $z = 2\Delta t d_t\xi^n$ in (3.19), sum over $1 \le n \le N-1$ and then estimate each term of the resulting equation. For the first two terms on the left-hand side of (3.19), one has

$$\begin{aligned}
&2\Delta t\sum_{n=1}^{N-1}[(s_1 d_t\xi^n, d_t\xi^n) + ((\bar{s}_1-s_1)(d_t\xi^n - d_t\xi^{n-1}), d_t\xi^n)]\\
&\qquad \ge\quad M\Delta t\sum_{n=1}^{N-1}\|d_t\xi^n\|^2 - \varepsilon\Delta t\|d_t\xi^0\|^2.
\end{aligned} \tag{3.20}$$

Here, in (3.20) and the rest of the proof, $\varepsilon > 0$ is a constant to be chosen sufficiently small later. For the third and fourth terms on the left-hand side of (3.19), we deduce that

$$\begin{aligned}
&\sum_{n=1}^{N-1}[(D\nabla\xi^n,\nabla d_t\xi^n) + \lambda\Delta t(s_1\nabla d_t\xi^n,\nabla d_t\xi^n)]\Delta t\\
&\quad =\quad \sum_{n=1}^{N-1}\{\frac{1}{2\Delta t}[(D\nabla\xi^{n+1},\nabla\xi^{n+1}) - (D\nabla\xi^n,\nabla\xi^n)]\\
&\qquad\qquad +\Delta t((\lambda s_1 - \frac{1}{2}D)\nabla d_t\xi^n,\nabla d_t\xi^n)\}\Delta t\\
&\quad \ge\quad D^*\|\nabla\xi^N\|^2 - D_*\|\nabla\xi^1\|^2 + (\lambda s_{1*} - \frac{1}{2}D^*)\sum_{n=1}^{N-1}\|\nabla d_t\xi^n\|^2\Delta t.
\end{aligned} \tag{3.21}$$

By the assumption that $\lambda > D^*/(2s_{1*})$, the coefficient of the last term of (3.21) is positive. The last two terms on the left-hand side of (1.3) can be bounded from below as follows:

$$(\lambda\Delta t)^2 \sum_{i\neq j,i,j=1}^{3} \left| \left(\bar{s}_1 \frac{\partial^2 d_t\xi^n}{\partial x_i \partial x_j}, \frac{\partial^2 d_t\xi^n}{\partial x_i \partial x_j} \right) \right| \geq M(\lambda\Delta t)^2 \sum_{i\neq j,i,j=1}^{3} \left\| \frac{\partial^2 d_t\xi^n}{\partial x_i \partial x_j} \right\|^2, \tag{3.22}$$

$$(\lambda\Delta t)^3 \left| \left(\bar{s}_1 \frac{\partial^3 d_t\xi^n}{\partial x_1 \partial x_2 \partial x_3}, \frac{\partial^3 d_t\xi^n}{\partial x_1 \partial x_2 \partial x_3} \right) \right| \geq M(\lambda\Delta t)^3 \left\| \frac{\partial^3 d_t\xi^n}{\partial x_1 \partial x_2 \partial x_3} \right\|^2. \tag{3.23}$$

It remains to estimate terms on the right-hand side of (3.19). We will bound these terms from above. We start with the first term on the right-hand side of (3.19). In view of (2.12), we have for sufficiently small h

$$|\Delta t \sum_{n=1}^{N-1} ((s_1^n - \bar{s}_1^n)\nabla d_t\xi^n, \nabla d_t\xi^n)| \leq \varepsilon \sum_{n=1}^{N-1} \|d_t\xi^n\|^2 \Delta t. \tag{3.24}$$

For the second term, the standard error estimates for difference quotients and the approximation property (2.17) for $\tilde{c}$ yield

$$2\Delta t \sum_{n=1}^{N-1} |((s_1^n - \bar{s}_1^n)(d_t\tilde{c}^n - d_t\tilde{c}^{n-1}), d_t\xi^n)| \leq \varepsilon \sum_{n=1}^{N-1} \|d_t\xi^n\|^2 \Delta t + M(\Delta t)^2. \tag{3.25}$$

To estimate the third term on the right-hand side of (3.19), let $F^n = \lambda\Delta t\bar{s}_1\nabla d_t\tilde{c}^n$. We have the identity

$$\begin{aligned} &2\Delta t \sum_{n=1}^{N-1} (F^n, \nabla d_t\xi^n) \\ &\quad = 2(F^{N-1}, \nabla\xi^N) - 2(F^1, \nabla\xi^1) - 2\Delta t \sum_{n=1}^{N-2} (d_t F^n, \nabla\xi^{n+1}). \end{aligned} \tag{3.26}$$

The terms on the right-hand side of (3.19) can be bounded by the Cauchy-Schwarz inequality and the approximation property (2.17) as follows:

$$\begin{aligned} &|(F^{N-1}, \nabla\xi^N) - (F^1, \nabla\xi^1)| \\ &\quad \leq \varepsilon\|\xi^N\|_1^2 + M\{\|F^{N-1}\|^2 + \|F^1\|^2 + \|\xi^1\|_1^2\} \\ &\quad \leq \varepsilon\|\xi^N\|_1^2 + M\{(\Delta t)^2\|d_t\tilde{c}^{N-1}\|_1^2 + (\Delta t)^2\|d_t\tilde{c}^1\|_1^2 + \|\xi^1\|_1^2\} \\ &\quad \leq \varepsilon\|\xi^N\|_1^2 + M\{(\Delta t)^2 + \|\xi^1\|_1^2\}, \end{aligned} \tag{3.27}$$

$$\begin{aligned} 2\Delta t \sum_{n=1}^{N-2} (d_t F^n, \nabla\xi^{n+1}) &\leq \varepsilon\Delta t \sum_{n=1}^{N-2} \|d_t F^n\|^2 + M\Delta t \sum_{n=1}^{N-2} \|\xi^{n+1}\|_1^2 \\ &\leq M\left\{ \sum_{n=2}^{N-1} \|\xi^n\|_1^2 \Delta t + (\Delta t)^2 \right\}. \end{aligned} \tag{3.28}$$

The identity (3.26) and the inequalities (3.27) and (3.28) give us the following upper bound for the third term on the right-hand side of (3.19):

$$\begin{aligned} &2\Delta t \sum_{n=1}^{N-1} (\lambda\Delta t\bar{s}_1\nabla d_t\tilde{c}^n, \nabla d_t\xi^n) \\ &\quad \leq \varepsilon\|\xi^N\|_1^2 + M\left((\Delta t)^2 + \|\xi^1\|_1^2 + \Delta t \sum_{n=2}^{N-1} \|\xi^n\|_1^2 \right). \end{aligned} \tag{3.29}$$

We now turn to the next term, the fourth term on the right-hand side of (3.19). Recall that

$$s_1 \frac{\partial c^{n+1}}{\partial t} + \mathbf{u}_h^n \cdot \nabla c^{n+1} = \psi(x, \mathbf{u}_h^n) \frac{\partial c^{n+1}}{\partial \tau},$$

where $\psi(x, \mathbf{u}_h^n) = (s_1^2(x) + |\mathbf{u}_h^n|^2)^{1/2}$. Let us make the induction hypothesis that

$$\sup_n \|\mathbf{u}_h^{n-1} - \tilde{\mathbf{u}}^{n-1}\|_{0,\infty} \le M. \tag{3.30}$$

By the induction hypothesis (3.30) we know that $\mathbf{u}_h^n$ is bounded, so is $\psi(x, \mathbf{u}_h^n)$. For Δt small enough, we have

$$\begin{aligned}
&\left\| s_1 \frac{\partial c^{n+1}}{\partial t} + \mathbf{u}_h^n \cdot \nabla c^{n+1} - s_1 \frac{c^{n+1} - \bar{c}^n}{\Delta t} \right\|^2 \\
=& \left\| \psi(x, \mathbf{u}_h^n) \frac{\partial c^{n+1}}{\partial \tau} - s_1 \frac{c^{n+1} - \bar{c}^n}{\Delta t} \right\|^2 \\
\le& \int_\Omega \left(\frac{s_1(x)}{\Delta t} \right)^2 \left(\frac{\psi \Delta t}{s_1(x)} \right)^3 \left| \int_{(\bar{x}, t^n)}^{(x, t^{n+1})} \frac{\partial^2 c}{\partial \tau^2} d\tau \right|^2 dx \\
\le& \Delta t \left\| \frac{\psi^3}{s_1} \right\|_{0,\infty} \int_\Omega \int_{t^n}^{t^{n+1}} \left| \frac{\partial^2 c}{\partial \tau^2} \right|^2 dt dx \\
\le& M(\Delta t) \left\| \frac{\partial^2 c}{\partial \tau^2} \right\|^2_{L^2(J^n; L^2)}.
\end{aligned}$$

Thus

$$\begin{aligned}
&\left| \left(s_1 \frac{\partial c^{n+1}}{\partial t} + \mathbf{u}_h^n \cdot \nabla c^{n+1} - s_1 \frac{c^{n+1} - \bar{c}^n}{\Delta t}, d_t \xi^n \right) \right| \\
&\le \varepsilon \sum_{n=1}^{N-1} \|d_t \xi^n\|^2 \Delta t + M(\Delta t)^2,
\end{aligned} \tag{3.31}$$

$$2\Delta t \sum_{n=1}^{N-1} \left(s_1 \frac{\bar{\xi}^n - \xi^n}{\Delta t}, d_t \xi^n \right) \le \varepsilon \sum_{n=1}^{N-1} \|d_t \xi^n\|^2 \Delta t + M \Delta t \sum_{n=1}^{N-1} \|\nabla \xi^n\|^2. \tag{3.32}$$

Note that

$$\left| \left(s_1 \frac{\eta^{n+1} - \bar{\eta}^n}{\Delta t}, d_t \xi^n \right) \right| \le \left| \left(s_1 \frac{\eta^{n+1} - \eta^n}{\Delta t}, d_t \xi^n \right) \right| + \left| \left(s_1 \frac{\eta^n - \bar{\eta}^n}{\Delta t}, d_t \xi^n \right) \right|.$$

It is easy to estimate the first term in the above equality. We will take diligent efforts on the following term:

$$\begin{aligned}
\Delta t \sum_{n=1}^{N-1} \left(s_1 \frac{\eta^n - \bar{\eta}^n}{\Delta t}, d_t \xi^n \right) &= \left(s_1 \frac{\eta^{N-1} - \bar{\eta}^{N-1}}{\Delta t}, \xi^N \right) \\
- \left(s_1 \frac{\eta^0 - \bar{\eta}^0}{\Delta t}, \xi^1 \right) &- \sum_{n=1}^{N-1} \left(s_1 \left(\frac{\eta^n - \bar{\eta}^n}{\Delta t} - \frac{\eta^{n-1} - \bar{\eta}^{n-1}}{\Delta t} \right), \xi^n \right).
\end{aligned} \tag{3.33}$$

It is easy to obtain:

$$\left| \left(s_1 \frac{\eta^{N-1} - \bar{\eta}^{N-1}}{\Delta t}, \xi^N \right) \right| \le \varepsilon \|\xi^N\|_1^2 + M \|\eta^{N-1}\|^2,$$

$$\left| \left(s_1 \frac{\eta^0 - \bar{\eta}^0}{\Delta t}, \xi^1) \right) \right| \le M \left\| \frac{\eta^0 - \bar{\eta}^0}{\Delta t} \right\|_{-1} \|\xi^1\|_1 \le M \{ h_s^{2l+2} + \|\xi^1\|_1^2 \}.$$

For the term

$$\begin{aligned}&\frac{\eta^n-\bar{\eta}^n}{\Delta t}-\frac{\eta^{n-1}-\bar{\eta}^{n-1}}{\Delta t}\\ &=\frac{1}{\Delta t}\left[\eta(x,t^n)-\eta(x,t^{n-1})-(\eta(\bar{x}^n,t^n)-\eta(\bar{x}^n,t^{n-1}))\right]\\ &-\frac{1}{\Delta t}\left[\eta(\bar{x}^n,t^n)-\eta(\bar{x}^{n-1},t^{n-1})\right]=I_1-I_2,\end{aligned} \tag{3.34}$$

using a Taylor expansion, we have $I_1=\int_0^1\left[\frac{\partial\eta}{\partial t}(x,t^\alpha)-\frac{\partial\eta}{\partial t}(\bar{x}^n,t^\alpha)\right]d\alpha$, where $t^\alpha=\alpha t^n+(1-\alpha)t^{n-1}$. Note that

$$\left\|\frac{\partial\eta}{\partial t}(x,t^\alpha)-\frac{\partial\eta}{\partial t}(\bar{x}^n,t^\alpha)\right\|_{-1}=\frac{1}{\|\phi\|_1}\sup_{\phi\in H^1(\Omega)}\int_\Omega\left[\frac{\partial\eta}{\partial t}(x,t^\alpha)-\frac{\partial\eta}{\partial t}(\bar{x}^n,t^\alpha)\right]\phi dx.$$

We introduce the space variant transformation $Z=F(x)=\bar{x}^n=x-\frac{u_h^n}{s_1(x)}\Delta t$, where DF represents the Jacobi matrix for transformation $Z=F(x)$ and $|det(DF)|$ be the Jacobi determinant for this transformation. For sufficiently small Δt, we have $|det(DF)|\le M\Delta t$ and $|det(DF)^{-1}|\le M\Delta t$. Similarly to the procedure in [6] we have the estimate:

$$\left\|\frac{\partial\eta}{\partial t}(x,t^\alpha)-\frac{\partial\eta}{\partial t}(\bar{x}^n,t^\alpha)\right\|_{-1}\le M\left\|\frac{\partial\eta}{\partial t}(t^\alpha)\right\|\Delta t.$$

Thus we have

$$\|I_1\|_{-1}\le M\Delta t\int_0^1\left\|\frac{\partial\eta}{\partial t}(t^\alpha)\right\|d\alpha. \tag{3.35}$$

To estimate I_2, we introduce the space variant transformation $Y=G(x)=\bar{x}^{n-1}=x-\frac{u_h^{n-1}}{s_1(x)}\Delta t$ to have

$$\begin{aligned}I_2&=\frac{1}{\Delta t}[\eta(\bar{x}^n,t^n)-\eta(\bar{x}^{n-1},t^{n-1})]\\ &=\frac{1}{\Delta t}\frac{1}{\|\phi\|_1}\sup_{\phi\in H^1(\Omega)}\int_\Omega\phi(x)[\eta(F(x),t^{n-1})-\eta(G(x),t^{n-1})]dx\\ &=\frac{1}{\Delta t}\frac{1}{\|\phi\|_1}\sup_{\phi\in H^1(\Omega)}\int_\Omega\phi(x)[\eta(Z,t^{n-1})-\eta(Y,t^{n-1})]dx\\ &=\frac{1}{\Delta t}\frac{1}{\|\phi\|_1}\sup_{\phi\in H^1(\Omega)}\{\int_\Omega\phi(F_{-1}(Z))\eta(Z,t^{n-1})det(DF)^{-1}(Z)dZ\\ &-\int_\Omega\phi(G^{-1}(Y))\eta(Y,t^{n-1})det(DG)^{-1}(Y)dY\},\end{aligned} \tag{3.36}$$

where

$$\begin{aligned}&\eta(Z,t^{n-1})[\phi(F^{-1}(Z))det(DF)^{-1}-\phi(G^{-1}(Z))det(DG)^{-1}]\\ &=\eta(Z,t^{n-1})\{\phi(F^{-1}(Z))[det(DF)^{-1}-det(DG)^{-1}]\\ &+det(DG)^{-1}[\phi(F^{-1}(Z))-\phi(G^{-1}(Z))]\}=A_1+A_2.\end{aligned} \tag{3.37}$$

Note that $\|\phi(F^{-1}(Z))\|\le M\|\phi\|$ and $|det(DF)^{-1}-det(DG)^{-1}|\le M(\Delta t)$. Then we have

$$A_1\le M\|\eta^{n-1}\|\Delta t, \tag{3.38}$$

$$
\begin{aligned}
|\phi(F^{-1}(Z)) - \phi(G^{-1}(Z))| &= \int_{G^{-1}(Z)}^{F^{-1}(Z)} \frac{\partial \phi}{\partial \beta}(\beta) d\beta \\
&= \int_0^1 \frac{\partial \phi}{\partial \beta}[G^{-1}(Z) + (F^{-1}(Z) - G^{-1}(Z))\theta](F^{-1}(Z) - G^{-1}(Z)) d\theta \\
&= \int_0^1 \frac{\partial \phi}{\partial \beta}(\theta)(F^{-1}(Z) - G^{-1}(Z)) d\theta.
\end{aligned} \tag{3.39}
$$

Since $|F^{-1}(Z) - G^{-1}(Z)| = |G^{-1}(Y) - G^{-1}(Z)| \leq |Y - Z| \leq M(\Delta t)$ and $|det(DG)^{-1}| \leq 1 + M\Delta t$, we see that

$$
A_2 \leq M\|\eta^{n-1}\|\Delta t. \tag{3.40}
$$

From (3.34) and (3.36) we obtain

$$
\|I_2\|_{-1} \leq M\|\eta^{n-1}\|\Delta t. \tag{3.41}
$$

Combining (3.30), (3.31) and (3.37), we have

$$
\begin{aligned}
&\sum_{n=1}^{N-1} \left(s_1 \left(\frac{\eta^n - \bar{\eta}^n}{\Delta t} - \frac{\eta^{n-1} - \bar{\eta}^{n-1}}{\Delta t} \right), \xi^n \right) \\
&\leq M(\Delta t)^{-1} \sum_{n=1}^{N-1} (\|I_1\|_{-1}^2 + \|I_2\|_{-1}^2) + M\Delta t \sum_{n=1}^{N-1} \|\xi^n\|_1^2 \\
&\leq M \sum_{n=1}^{N-1} \left\{ \left\|\eta^{n-1}\right\|^2 + \int_0^1 \left\| \frac{\partial \eta}{\partial t}(t^\alpha) \right\|^2 d\alpha \right\} \Delta t + M\Delta t \sum_{n=1}^{N-1} \|\xi^n\|_1^2 \\
&\leq M \left\{ h_s^{2l+2} + (\Delta t)^2 + \Delta t \sum_{n=1}^{N-1} \|\xi^n\|_1^2 \right\}.
\end{aligned} \tag{3.42}
$$

For the other terms on the right-hand side of (3.17), when $l \geq 1$, we have

$$
\left| \sum_{i \neq j, i,j=1}^{3} \left(s_1 \frac{\partial^2 d_t \tilde{c}^n}{\partial x_i \partial x_j}, \frac{\partial^2 \xi^{n+1}}{\partial x_i \partial x_j} \right) \right| \leq M(\Delta t)^2 + \varepsilon(\lambda \triangle t)^2 \sum_{i \neq j, i,j=1}^{3} \left\| \frac{\partial^2 \xi^{n+1}}{\partial x_i \partial x_j} \right\|^2
$$

and when $l \geq 1, \Delta t = O(h_c^2)$, we get

$$
\left| \left(s_1 \frac{\partial^3 d_t \tilde{c}^n}{\partial x_1 \partial x_2 \partial x_3}, \frac{\partial^3 \xi^{n+1}}{\partial x_1 \partial x_2 \partial x_3} \right) \right| \leq M(\Delta t)^2 + \varepsilon(\lambda \triangle t)^3 \left\| \frac{\partial^3 \xi^{n+1}}{\partial x_1 \partial x_2 \partial x_3} \right\|^2.
$$

The other terms can be estimated easily:

$$
\begin{aligned}
&\sum_{n=1}^{N-1} \|d_t \xi^n\|^2 \Delta t + \|\xi^N\|_1^2 \\
&\leq M \left\{ \sum_{n=1}^{N-1} \|\xi^n\|_1^2 (\Delta t) + (\Delta t)^2 + h_p^{2k+2} + h_s^{2l+2} + h_c^{2r+2} \right\} + \|\xi^1\|_1^2.
\end{aligned} \tag{3.43}
$$

We next combine (3.15) and (3.39), and choose ε sufficiently small to obtain

$$
\begin{aligned}
&\|\rho^N\|^2 + \|\xi^N\|_1^2 + \sum_{n=1}^{N-1} \|d_t \xi^n\|^2 \Delta t \\
&\leq M\{(\Delta t)^2 + h_p^{2k+2} + h_c^{2l+2} + h_c'^{2r+2}\} + \sum_{n=0}^{N-1} (\|\xi^n\|_1^2 + \|\rho^{n+1}\|^2)\Delta t.
\end{aligned} \tag{3.44}
$$

If condition (3.9) holds, an application of a discrete version of Gronwall's lemma shows that

$$\begin{aligned} &\|\xi^N\|_1^2 + \|\rho^N\|^2 + \sum_{n=0}^{N-1} \|d_t\xi^n\|^2 \Delta t \\ &\leq M\{(\Delta t)^2 + h_p^{2k+2} + h_c^{2l+2} + h_c'^{2r+2}\}. \end{aligned} \tag{3.45}$$

Now, check the induction hypothesis (3.26) and suppose $k \geq 1, l \geq 1$; then, under the constraint (3.8), the induction hypothesis (3.26) holds.

We can summarize our results by combining (3.3), (3.5), (3.7) and (3.41). □

4. Start-up procedure

For the three-level method (2.12), one must obtain C^0, C^1 and C'^0, C'^1 such that (3.9) holds. Ideally, we choose $C^0 = \tilde{c}(0)$, $C'^0 = \tilde{c}'(0)$. If the linear system associated with $\tilde{c}(0)$ or $\tilde{c}'(0)$ cannot be solved exactly, an iterative procedure such as a preconditioned conjugate-gradient method may be used to obtain C^0 and C'^0 close to $\tilde{c}(0)$ and $\tilde{c'}(0)$ separately.

We obtain u_h^0 by solving the following equations:

$$(a(C^0)^{-1}\mathbf{u}_h^0, \mathbf{v}) - (\nabla \cdot \mathbf{v}, p_h^0) = 0, \quad \mathbf{v} \in V_h,$$
$$(\nabla \cdot \mathbf{u}_h^0, \varphi) = (q, \varphi), \quad \varphi \in W_h.$$

We can obtain C'^1 by solving (2.13). There are several possible methods for obtaining C^1. We can define C^1 with one iteration by

$$(s_1 \frac{C^1 - \bar{C}^0}{\triangle t}, z) + (D\nabla C^1, \nabla z) + (s_2 \frac{C'^1 - C'^0}{\triangle t}, z) = (q(C^{*0} - C^0), z), \quad z \in M_h,$$

where $\bar{C}^0 = C(x - \dfrac{\mathbf{u}_h^0}{s_1(x)} \triangle t)$.

One can also obtain C^1 by defining the following iterative procedure, whose matrix factors into the alternating-direction form

$$Y^0 = C^0 = \tilde{c}(0),$$

$$\begin{aligned} &\left(\bar{s}_1 \frac{Y^{i+1} - C^0}{\Delta t}, z\right) + (s_2 d_t C'^n, z) + (D\nabla C^0, \nabla z) \\ &+\lambda \left(\bar{s}_1(\nabla(Y^{i+1} - C^0)), \nabla z\right) + \lambda^2 \Delta t \sum_{i\neq j, i,j=1}^{3} \left(\bar{s}_1 \frac{\partial^2(Y^{i+1} - C^0)}{\partial x_i \partial x_j}, \frac{\partial^2 z}{\partial x_i \partial x_j}\right) \\ &+\lambda^3 \Delta t^2 \left(\bar{s}_1 \frac{\partial^3(Y^{i+1} - C^0)}{\partial x_1 \partial x_2 \partial x_3}, \frac{\partial^3 z}{\partial x_1 \partial x_2 \partial x_3}\right) \\ &= (q(C^{*0} - C^0), z) + ((\bar{s}_1 - s_1)\frac{Y^{i+1} - C^0}{\triangle t}, z) - (s_1 \frac{C^0 - \bar{C}^0}{\triangle t}, z), \quad z \in M_h. \end{aligned}$$

It is straightforward to verify that this choice of C^0, C^1 and C'^0, C'^1 satisfies the hypothesis of Theorem 3.1.

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