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A Conservative Upwind Approximation on Block-Centered Difference for Chemical Oil Recovery Displacement Problem

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Abstract. A kind of conservative upwind method is discussed for chemical oil recovery displacement in porous media. The mathematical model is formulated by a nonlinear convection-diffusion system dependent on the pressure, Darcy velocity, concentration and saturations. The flow equation is solved by a conservative block-centered method, and the pressure and Darcy velocity are obtained at the same time. The concentration and saturations are determined by convection-dominated diffusion equations, so an upwind approximation is adopted to eliminate numerical dispersion and nonphysical oscillation. Block-centered method is conservative locally. An upwind method with block-centered difference is used for computing the concentration. The saturations of different components are solved by the method of upwind fractional step difference, and the computational work is shortened significantly by dividing a three-dimensional problem into three successive one-dimensional problems and using the method of speedup. Using the variation discussion, energy estimates, the method of duality, and the theory of a priori estimates, we complete numerical analysis. Finally, numerical tests are given for showing the computational accuracy, efficiency and practicability of our approach.

AMS subject classifications: 65N12, 65N30, 65M12, 65M15

Key words: Chemical oil recovery, upwind block-centered difference, fractional step difference, elemental conservation, convergence analysis.

1 Introduction

Oil exploration plays an important rule in industrial engineering fields, while the underground crude oil becomes less. New challenges of exploration techniques appear in

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this project, such as how to decrease the cost and increase the recovery efficiency at the present oilfields. At present, a new recovery technique, chemical agents used during the displacement, is generalized. Under the influences of driving fluids with addition of chemical agents, crude oil is migrated and accumulated easily through the underground media. Some chemical additives usually include polymer, surface active agent and alkali. This is called "chemical oil recovery" [1–6]. The mathematical model is formulated by a nonlinear system of partial differential equations [7–11]. It is important to find efficient numerical methods for simulating how the underground fluids flow and oil is displaced more accurately. In this paper, the physical natures and the characters of mathematical model are considered carefully, then a kind of upwind method with block-centered difference and fractional step difference together is discussed. Numerical analysis and experimental tests are shown.

The mathematical model with initial-boundary conditions is given

$$-\nabla\cdot\Big(\frac{\kappa(X)}{\mu(c)}\nabla p\Big)\equiv\nabla\cdot\mathbf{u}=q(X,t)=q_I+q_p,\quad X=(x,y,z)^T\in\Omega,\quad t\in J=(0,T],\tag{1.1a}$$

$$\mathbf{u}=-\frac{\kappa(X)}{\mu(c)}\nabla p,\qquad X\in\Omega,\qquad t\in J,\tag{1.1b}$$

and

$$\phi\frac{\partial c}{\partial t}+\mathbf{u}\cdot\nabla c-\nabla\cdot(D(\mathbf{u})\nabla c)+q_I c=q_I c_I,\qquad X\in\Omega,\quad t\in J,\tag{1.2a}$$

$$\phi\frac{\partial}{\partial t}(cs_\alpha)+\nabla\cdot(s_\alpha\mathbf{u}-\phi c\kappa_\alpha\nabla s_\alpha)=Q_\alpha(X,t,c,s_\alpha),\quad X\in\Omega,\quad t\in J,\quad \alpha=1,2,\cdots,n_c,\tag{1.2b}$$

where Ω is a bounded domain in R^3. The pressure, Darcy velocity, the concentration of water and the saturations of different chemical components are denoted by $p(X,t)$, $\mathbf{u}=(u_1,u_2,u_3)^T$, $c(X,t)$ and s_α ($\alpha=1,\cdots,n_c$) respectively. Other major parameters are interpreted as follows

- $q(X,t)$, the quantity, usually defined by the production q_p and the injection q_I, i.e.,
$$q(X,t)=q_I(X,t)+q_p(X,t),$$
- c_I, the concentration of injected fluid,
- $\phi(X)$, the porosity of rock,
- $\kappa(X)$, the absolute permeability,
- $\mu(c)$, the viscosity of mixture dependent on c,
- $D=D(\mathbf{u})$, the diffusion coefficient, defined by molecular diffusion and mechanical dispersion
$$\mathbf{D}(X,\mathbf{u})=\phi d_m\mathbf{I}+|\mathbf{u}|^\beta\begin{pmatrix} d_l & 0 & 0\\ 0 & d_t & 0\\ 0 & 0 & d_t\end{pmatrix}=\begin{pmatrix} d_x(\mathbf{u}) & 0 & 0\\ 0 & d_y(\mathbf{u}) & 0\\ 0 & 0 & d_z(\mathbf{u})\end{pmatrix},\tag{1.3}$$

- d_m, the molecular diffusivity,
- $\mathbf{I}$, a 3×3 identity matrix,
- d_l, the longitudinal dispersivity,
- d_t, the transverse dispersivity,
- n_c, the number of components,
- $\kappa_\alpha=\kappa_\alpha(X)$, the diffusion of α-component,
- Q_α, the source and sink term.

Initial-boundary conditions of (1.1)–(1.2b) are defined by

$$\begin{aligned}
&\mathbf{u}\cdot\gamma=0, \quad (D(\mathbf{u})\nabla c-\mathbf{u}c)\cdot\gamma=0, && X\in\partial\Omega, \quad t\in J, && (1.4a)\\
&s_\alpha=h_\alpha(X,t), && X\in\partial\Omega, \quad t\in J, \quad \alpha=1,2,\cdots,n_c, && (1.4b)\\
&c(X,0)=c_0(X), && X\in\Omega, && (1.4c)\\
&s_\alpha(X,0)=s_{\alpha,0}(X), && X\in\Omega, \quad \alpha=1,2,\cdots,n_c, && (1.4d)
\end{aligned}$$

where γ denotes a unit outward normal vector to $\partial\Omega$, the boundary of Ω.

To avoid the ambiguity, we introduce the following constraints

$$\int_\Omega q(X,t)dX=0, \quad \int_\Omega p(X,t)dX=0, \quad t\in J. \tag{1.5}$$

Using (1.1) and (1.2a), we reformulate (1.2b) as follow

$$\begin{aligned}
&\phi c\frac{\partial s_\alpha}{\partial t}+\mathbf{u}\cdot\nabla s_\alpha-\nabla\cdot(\phi c\kappa_\alpha\nabla s_\alpha)\\
=&Q_\alpha-s_\alpha\Big(q+\phi\frac{\partial c}{\partial t}\Big), \quad X\in\Omega, \quad t\in J, \quad \alpha=1,2,\cdots,n_c.
\end{aligned} \tag{1.6}$$

Oil recovery is an open international problem, and numerical simulation of underground oil-water gives helpful suggestions on locating oilfields and exploration. The original research is discussed by Douglas, Ewing, Wheeler and other scholars [1,7–11]. Yuan and his academic team present some stable and efficient numerical methods, and apply these on actual productions in Shengli Oilfield [2–6, 11–13]. At present, a new stage (chemical oil recovery) is necessary. Some chemical addition agents are used for enforcing the flooding and increasing recovery efficiency of existing oilfields. The mathematical model of this problem has the convection-dominated property and conservative nature. Furthermore, its numerical simulations run on a wide region and a long time. For convection-dominated diffusion equations, some traditional numerical methods such as finite difference and finite element give rise to numerical dispersion or nonphysical oscillation. Thus, some new techniques appear. Douglas, Ewing, Russell, Wheeler and other scholars present the method of characteristics (MOC) and give some improved schemes [8–10].

Ewing and Lazarov put forward an upwind difference (UD) [14,15]. MOC and UD could solve the convection-diffusion equations well. MOC introduces some additional computations at the boundary that makes the whole computation more complicated. In actual applications, the UD becomes more popular.

Finite volume element method (FVE) shows the simplicity, high accuracy, and the local conservation of mass in [16,17], therefore it is motivated to become a powerful tool to solve partial differential equations. The mixed finite element method (MFE) could solve the pressure and Darcy velocity simultaneously, and could achieve accuracy of the first order in [18–20]. Combined FVE and MFE, a block-centered difference (BCD) is discussed in [21,22] and computational validity is shown by experimental tests in [23,24]. A block-centered scheme and its convergence analysis are discussed for elliptic problems in [25–27], then a frame work of its theory and application is shown. Rui and his research group show a series work of this method to discuss numerical computation for Darcy-Forchheimer flow problems in [28–33]. The authors apply this method to solve numerical simulation of semiconductor device and the problem is approximated well [34,35].

For large-scaled computations, Lions and Peaceman put forward an alternating direction scheme [36, 37], while theoretical analysis is not shown. Marchuk and Yanenko give the basic work on fractional step differences (FSD) [38, 39], and computational efficiency is discussed. The whole computation on a three-dimensional region is divided into three successive one-dimensional problems so that the computational work is decreased greatly, where the speedup solver is used [12, 37]. Some composite procedures of UD and FSD are discussed and applied in actual productions [4,12,40–42]. Based on the previous studies, an upwind block-centered fractional step difference method (UBCFSD) is proposed for simulating a three-dimensional chemical oil recovery problem in this paper. The pressure and Darcy velocity are computed simultaneously by the BCD, and the accuracy is improved by one order for the Darcy velocity. The concentration is computed by using an upwind block-centered difference (UBCD), where the convection and diffusion are approximated by the UD and BCD, respectively. The composite combination method eliminates numerical dispersion and can solve convection-dominated diffusion problem with high accuracy. We apply the block-centered scheme to address diffusion and obtain the values of the unknown concentration and adjoint vector simultaneously. The composite combination scheme is locally conservative, an important nature in numerical simulation of chemical oil recovery seepage mechanics. The saturations of different components, whose computational work is the largest, are treated by upwind fractional step differences. Applying the variation form, energy error estimates, duality discussion and the theory of a priori estimates, we complete numerical analysis. Finally, numerical experiments are given for a similar nonlinear system, illustrating high computational efficiency and theoretical results. Therefore, this presented method possibly provides an efficient tool for solving such a challenging problem [1,6,7,11,44].

The notation and norms of Sobolev space are adopted in this paper. The regularity assumptions of (1.1)-(1.5) are defined by

$$
\text{(R)} \qquad \begin{cases} p \in L^\infty(H^1), \\ \mathbf{u} \in L^\infty(H^1(\mathrm{div})) \bigcap L^\infty(W^1_\infty) \bigcap W^1_\infty(L^\infty) \bigcap H^2(L^2), \\ c, s_\alpha \in L^\infty(H^2) \bigcap H^1(H^1) \bigcap L^\infty(W^1_\infty) \bigcap H^2(L^2), \quad \alpha = 1,2,\cdots,n_c. \end{cases}
$$

We suppose that the coefficients of (1.1)-(1.5) satisfy the following positive definite conditions

$$
\text{(C)} \qquad \begin{cases} 0 < a_* \le \dfrac{\kappa(X)}{\mu(c)} \le a^*, \quad 0 < \phi_* \le \phi(X) \le \phi^*, \quad 0 < D_* \le D(X,\mathbf{u}), \\ 0 < K_* \le \kappa_\alpha(X,t) \le K^*, \quad \alpha = 1,2,\cdots,n_c, \end{cases}
$$

where a_*, a^*, ϕ_*, ϕ^*, D_*, K_* and K^* are positive constants.

This paper is organized as follows. In Section 1, the mathematical model is stated, and the physical background and related research are introduced. In Section 2, three partitions and preliminary statements are stated. In Section 3, the authors propose the method of UBCFSD. The flow equation is treated by a conservative BCD, and an approximation of the Darcy velocity with one-order improvement is shown. The UBCD method is applied to solve the concentration equation, where the convection is assessed by the method of BCD and the diffusion is approximated by the UD scheme. The upwind technique can solve convection-dominated diffusion equations well because it avoids numerical dispersion and nonphysical oscillation and confirms high accuracy. The BCD scheme can compute the concentration and its adjoint vector function simultaneously. It is elementally conservative. The saturations of different components are computed by the method of upwind fractional step difference in parallel, where the whole computation is divided into three one-dimensional problems and the simple speedup solver is used. In Section 4, an optimal order error estimates is concluded. In Section 5, numerical examples are discussed to illustrate theoretical analysis and show the feasibility of the presented composite scheme.

In the following discussions, the symbols K and ε denote a generic positive constant and a generic small positive number, respectively. They have different definitions at different places.

2 Notation and preparations

Numerical model includes four major partial differential equations determining the pressure, Darcy velocity, concentration and saturations. Considering the natures of mathematical model, three partitions with different sizes are given. Suppose that the partitions are regular. First, the concentration and saturations change more faster than pressure and Darcy velocity. The partition with large step is for the flow equation. The middle-size partition is for the concentration. For interpreting the effects of the chemical addition agents during the flooding process, the saturations are computed on the small-size mesh. Thus, the computation work is the largest.

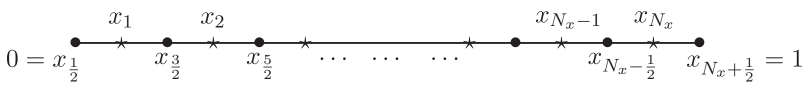

Figure 1: The partition of δ_x.

Without loss of generality, take $\Omega=\{[0,1]\}^3$ with the boundary $\partial\Omega$. For $x\in[0,1]$, define its partition δ_x (see Fig. 1)

$$\delta_x:\ 0=x_{1/2}<x_{3/2}<\cdots<x_{N_x-1/2}<x_{N_x+1/2}=1.$$

Other partitions

$$\begin{aligned}&\delta_y:\ 0=y_{1/2}<y_{3/2}<\cdots<y_{N_y-1/2}<y_{N_y+1/2}=1,\\&\delta_z:\ 0=z_{1/2}<z_{3/2}<\cdots<z_{N_z-1/2}<z_{N_z+1/2}=1,\end{aligned}$$

are defined similarly. N_x, N_y and N_z are three positive integers, denoting the numbers of nodes in three directions. Ω is partitioned by $\delta_x\times\delta_y\times\delta_z$. Let

$$\begin{aligned}&\Omega_{ijk}=\big\{(x,y,z)|x_{i-1/2}<x<x_{i+1/2},\, y_{j-1/2}<y<y_{j+1/2},\, z_{k-1/2}<z<z_{k+1/2}\big\},\\&x_i=(x_{i-1/2}+x_{i+1/2})/2,\quad h_{x_i}=x_{i+1/2}-x_{i-1/2},\\&h_{x,i+1/2}=x_{i+1}-x_i,\quad h_x=\max_{1\le i\le N_x}\{h_{x_i}\}.\end{aligned}$$

The symbols y_j, z_k, h_{y_j}, h_{z_k}, $h_{y,j+1/2}$, $h_{z,k+1/2}$, h_y and h_z are defined similarly. Let

$$h_p=(h_x^2+h_y^2+h_z^2)^{1/2}\quad\text{and}\quad I_i^x=[x_{i-1/2},x_{i+1/2}],$$

then define

$$M_l^d(\delta_x)=\{f\in C^l[0,1]:\ f|_{I_i^x}\in p_d(I_i^x),\ i=1,2,\cdots,N_x\}.$$

$p_d(I_i^x)$ denotes a space consisting of all the polynomial functions of degree at most d constricted on I_i^x. $f(x)$ is possibly discontinuous on $[0,1]$ as $l=-1$. $M_l^d(\delta_y)$ and $M_l^d(\delta_z)$ are defined similarly. Let

$$\begin{aligned}&S_h=M_{-1}^0(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_{-1}^0(\delta_z),\\&V_h=\{\mathbf{w}|\mathbf{w}=(w^x,w^y,w^z),\ w^x\in M_0^1(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_{-1}^0(\delta_z),\\&\qquad w^y\in M_{-1}^0(\delta_x)\bigotimes M_0^1(\delta_y)\bigotimes M_{-1}^0(\delta_z),\ w^z\in M_{-1}^0(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_0^1(\delta_z),\\&\qquad \mathbf{w}\cdot\gamma|_{\partial\Omega}=0\}.\end{aligned}$$

Define the inner products and norms by

$$\begin{aligned}
&(v,w)_{\bar{m}}=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_i}h_{y_j}h_{z_k}v_{ijk}w_{ijk},\\
&(v,w)_x=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_{i-1/2}}h_{y_j}h_{z_k}v_{i-1/2,jk}w_{i-1/2,jk},\\
&(v,w)_y=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_i}h_{y_{j-1/2}}h_{z_k}v_{i,j-1/2,k}w_{i,j-1/2,k},\\
&(v,w)_z=\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}h_{x_i}h_{y_j}h_{z_{k-1/2}}v_{ij,k-1/2}w_{ij,k-1/2},\\
&||v||_s^2=(v,v)_s,\quad s=\bar{m},x,y,z,\quad ||v||_\infty=\max_{1\le i\le N_x,1\le j\le N_y,1\le k\le N_z}|v_{ijk}|,\\
&||v||_{\infty(x)}=\max_{1\le i\le N_x,\ 1\le j\le N_y,\ 1\le k\le N_z}|v_{i-1/2,jk}|,\\
&||v||_{\infty(y)}=\max_{1\le i\le N_x,\ 1\le j\le N_y,\ 1\le k\le N_z}|v_{i,j-1/2,k}|,\\
&||v||_{\infty(z)}=\max_{1\le i\le N_x,\ 1\le j\le N_y,\ 1\le k\le N_z}|v_{ij,k-1/2}|.
\end{aligned}$$

For a vector $\mathbf{w}=(w^x,w^y,w^z)^T$, define its norms by

$$\begin{aligned}
&|||\mathbf{w}|||=\Big(||w^x||_x^2+||w^y||_y^2+||w^z||_z^2\Big)^{1/2},\quad |||\mathbf{w}|||_\infty=||w^x||_{\infty(x)}+||w^y||_{\infty(y)}+||w^z||_{\infty(z)},\\
&||\mathbf{w}||_{\bar{m}}=\big(||w^x||_{\bar{m}}^2+||w^y||_{\bar{m}}^2+||w^z||_{\bar{m}}^2\big)^{1/2},\quad ||\mathbf{w}||_\infty=||w^x||_\infty+||w^y||_\infty+||w^z||_\infty.
\end{aligned}$$

Define

$$\begin{aligned}
W_p^m(\Omega)=\Big\{v\in L^p(\Omega)\Big|&\frac{\partial^n v}{\partial x^{n-l-r}\partial y^l\partial z^r}\in L^p(\Omega),\ n-l-r\ge 0,\ l=0,1,\cdots,n;\\
&r=0,1,\cdots,n,\ n=0,1,\cdots,m;\ 0<p<\infty\},
\end{aligned}$$

and let

$$H^m(\Omega)=W_2^m(\Omega).$$

Inner product and norm in $L^2(\Omega)$ are denoted by $(\cdot,\cdot)$ and $||\cdot||$. For a function $v\in S_h$, it clearly holds that

$$||v||_{\bar{m}}=||v||. \tag{2.1}$$

Introduce the difference operators and other notation as follows,

$$[d_x v]_{i+1/2,jk}=\frac{v_{i+1,jk}-v_{ijk}}{h_{x,i+1/2}}, \qquad [d_y v]_{i,j+1/2,k}=\frac{v_{i,j+1,k}-v_{ijk}}{h_{y,j+1/2}},$$
$$[d_z v]_{ij,k+1/2}=\frac{v_{ij,k+1}-v_{ijk}}{h_{z,k+1/2}}, \qquad [D_x w]_{ijk}=\frac{w_{i+1/2,jk}-w_{i-1/2,jk}}{h_{x_i}},$$
$$[D_y w]_{ijk}=\frac{w_{i,j+1/2,k}-w_{i,j-1/2,k}}{h_{y_j}}, \qquad [D_z w]_{ijk}=\frac{w_{ij,k+1/2}-w_{ij,k-1/2}}{h_{z_k}},$$
$$\hat{w}^x_{ijk}=\frac{w^x_{i+1/2,jk}+w^x_{i-1/2,jk}}{2}, \qquad \hat{w}^y_{ijk}=\frac{w^y_{i,j+1/2,k}+w^y_{i,j-1/2,k}}{2},$$
$$\hat{w}^z_{ijk}=\frac{w^z_{ij,k+1/2}+w^z_{ij,k-1/2}}{2}, \qquad \bar{w}^x_{ijk}=\frac{h_{x,i+1}}{2h_{x,i+1/2}}w_{ijk}+\frac{h_{x,i}}{2h_{x,i+1/2}}w_{i+1,jk},$$
$$\bar{w}^y_{ijk}=\frac{h_{y,j+1}}{2h_{y,j+1/2}}w_{ijk}+\frac{h_{y,j}}{2h_{y,j+1/2}}w_{i,j+1,k}, \qquad \bar{w}^z_{ijk}=\frac{h_{z,k+1}}{2h_{z,k+1/2}}w_{ijk}+\frac{h_{z,k}}{2h_{z,k+1/2}}w_{ij,k+1},$$
$$\hat{\mathbf{w}}_{ijk}=(\hat{w}^x_{ijk},\hat{w}^y_{ijk},\hat{w}^z_{ijk})^T, \qquad \bar{\mathbf{w}}_{ijk}=(\bar{w}^x_{ijk},\bar{w}^y_{ijk},\bar{w}^z_{ijk})^T,$$

and $d_s(s=x,y,z)$ and $D_s(s=x,y,z)$ are difference quotient operators independent of the coefficient D in (1.2a). Let L denote a positive integer, $\Delta t=T/L$, $t^n=n\Delta t$, $v^n=v(t^n)$ and $d_t v^n=(v^n-v^{n-1})/\Delta t$.

Based on the above notation, several preliminary statements can be given.

Lemma 2.1. *For $v\in S_h$, $\mathbf{w}\in V_h$, we have*

$$(v,D_x w^x)_{\bar{m}}=-(d_x v,w^x)_x, \quad (v,D_y w^y)_{\bar{m}}=-(d_y v,w^y)_y, \quad (v,D_z w^z)_{\bar{m}}=-(d_z v,w^z)_z. \tag{2.2}$$

Lemma 2.2. *For $\mathbf{w}\in V_h$, we have*

$$||\hat{\mathbf{w}}||_{\bar{m}}\le |||\mathbf{w}|||. \tag{2.3}$$

Lemma 2.3. *For $q\in S_h$,*

$$||\bar{q}^x||_x\le M||q||_{\bar{m}}, \quad ||\bar{q}^y||_y\le M||q||_{\bar{m}}, \quad ||\bar{q}^z||_z\le M||q||_{\bar{m}}, \tag{2.4}$$

where M is a constant independent of q and h.

Lemma 2.4. *For $\mathbf{w}\in V_h$,*

$$||w^x||_x\le ||D_x w^x||_{\bar{m}}, \quad ||w^y||_y\le ||D_y w^y||_{\bar{m}}, \quad ||w^z||_z\le ||D_z w^z||_{\bar{m}}. \tag{2.5}$$

The middle-size partition is obtained by refining the large-size partition of $\Omega=\{[0,1]\}^3$ uniformly. Generally, take $h_c=h_p/2$ or $h_c=h_p/4$. Other notation is defined as above.

The small-size partition of $\Omega=\{[0,1]\}^3$ is defined uniformly,

$$\bar{\delta}_x:\ 0=x_0<x_1<\cdots<x_{M_1-1}<x_{M_1}=1,$$
$$\bar{\delta}_y:\ 0=y_0<y_1<\cdots<y_{M_2-1}<y_{M_2}=1,$$
$$\bar{\delta}_z:\ 0=z_0<z_1<\cdots<z_{M_3-1}<z_{M_3}=1,$$

where M_1, M_2 and M_3 are positive constants. The space steps and other notation are denoted by

$$\begin{aligned} &h^x=\frac{1}{M_1}, && h^y=\frac{1}{M_2}, && h^z=\frac{1}{M_3},\\ &x_i=i\cdot h^x, && y_j=j\cdot h^y, && z_k=k\cdot h^z,\\ &h_s=((h^x)^2+(h^y)^2+(h^z)^2)^{1/2}. \end{aligned}$$

Let

$$D_{i+1/2,jk}=\frac{1}{2}[D(X_{ijk})+D(X_{i+1,jk})],\quad D_{i-1/2,jk}=\frac{1}{2}[D(X_{ijk})+D(X_{i-1,jk})],$$

and define $D_{i,j+1/2,k}$, $D_{i,j-1/2,k}$, $D_{ij,k+1/2}$, $D_{ij,k-1/2}$ similarly. Define

$$\delta_{\bar{x}}(D\delta_x W)^n_{ijk}=(h^x)^{-2}[D_{i+1/2,jk}(W^n_{i+1,jk}-W^n_{ijk})-D_{i-1/2,jk}(W^n_{ijk}-W^n_{i-1,jk})], \tag{2.6a}$$

$$\delta_{\bar{y}}(D\delta_y W)^n_{ijk}=(h^y)^{-2}[D_{i,j+1/2,k}(W^n_{i,j+1,k}-W^n_{ijk})-D_{i,j-1/2,k}(W^n_{ijk}-W^n_{i,j-1,k})], \tag{2.6b}$$

$$\delta_{\bar{z}}(D\delta_z W)^n_{ijk}=(h^z)^{-2}[D_{ij,k+1/2}(W^n_{ij,k+1}-W^n_{ijk})-D_{ij,k-1/2}(W^n_{ijk}-W^n_{ij,k-1})], \tag{2.6c}$$

$$\nabla_h(D\nabla W)^n_{ijk}=\delta_{\bar{x}}(D\delta_x W)^n_{ijk}+\delta_{\bar{y}}(D\delta_y W)^n_{ijk}+\delta_{\bar{z}}(D\delta_z W)^n_{ijk}. \tag{2.6d}$$

3 The procedures of upwind block-centered fractional step differences

3.1 The procedures

We rewrite (1.1) as the following normal formulation to clarify the block-centered method

$$\nabla\cdot\mathbf{u}=q, \tag{3.1a}$$

$$\mathbf{u}=-a(c)\nabla p, \tag{3.1b}$$

where $a(c)=\kappa(X)\mu^{-1}(c)$.

The concentration equation (1.2a) is rewritten in a divergent form to construct the computational scheme. Let

$$\mathbf{g}=\mathbf{u}c=(u_1c,u_2c,u_3c)^T,\quad \bar{\mathbf{z}}=-\nabla c\quad\text{and}\quad \mathbf{z}=D\bar{\mathbf{z}}.$$

Then,

$$\phi\frac{\partial c}{\partial t}+\nabla\cdot\mathbf{g}+\nabla\cdot\mathbf{z}-c\nabla\cdot\mathbf{u}=q_I(c_I-c). \tag{3.2}$$

Using the fact that $\nabla\cdot\mathbf{u}=q=q_I+q_p$, we have

$$\phi\frac{\partial c}{\partial t}+\nabla\cdot\mathbf{g}+\nabla\cdot\mathbf{z}-q_pc=q_Ic_I. \tag{3.3}$$

Here we adopt the expanded block-centered method [45] to obtain the approximations of $\mathbf{z}$ and $\bar{\mathbf{z}}$ simultaneously.

A large time step, denoted by Δt_p, is adopted for the pressure and a small time step Δt_c for the concentration and saturations. Let $\Delta t_{p,1}$ denote the first time step. The time interval $J=[0,T]$ is partitioned by $0=t_0<t_1<\cdots<t_M=T$, where $t_i=\Delta t_{p,1}+(i-1)\Delta t_p$ for $i\geq 1$. Similarly, another partition is defined by $0=t^0<t^1<\cdots<t^N=T$ for the concentration and $t^n=n\Delta t_c$. Suppose that there exists a positive integer n such that $t_m=t^n$ for any number m, that is, $\frac{\Delta t_p}{\Delta t_c}$ is a positive integer. Let

$$j_0^*=\Delta t_{p,1}/\Delta t_c \quad \text{and} \quad j^*=\Delta t_p/\Delta t_c.$$

Let P, $\mathbf{U}$, C, $\mathbf{G}$, $\mathbf{Z}$ and $\bar{\mathbf{Z}}$ denote numerical solutions of p, $\mathbf{u}$, c, $\mathbf{g}$, $\mathbf{z}$ and $\bar{\mathbf{z}}$ in $S_h\times V_h\times S_h\times V_h\times V_h\times V_h$. Based on the notation and preliminary statements in Section 2, a block-centered scheme is defined for simulating the pressure and Darcy velocity,

$$\begin{aligned}
&\big(D_xU_m^x+D_yU_m^y+D_zU_m^z,v\big)_{\bar{m}}=(q_m,v)_{\bar{m}}, && \forall v\in S_h, && \text{(3.4a)}\\
&\Big(a^{-1}(\bar{C}_m^x)U_m^x,w^x\Big)_x+\Big(a^{-1}(\bar{C}_m^y)U_m^y,w^y\Big)_y+\Big(a^{-1}(\bar{C}_m^z)U_m^z,w^z\Big)_z\\
&\quad-(P_m,D_xw^x+D_xw^y+D_xw^z)_{\bar{m}}=0, && \forall \mathbf{w}\in V_h. && \text{(3.4b)}
\end{aligned}$$

The variational form of (3.3) is

$$\begin{aligned}
&\Big(\phi\frac{\partial c}{\partial t},v\Big)_{\bar{m}}+(\nabla\cdot\mathbf{g},v)_{\bar{m}}+(\nabla\cdot\mathbf{z},v)_{\bar{m}}-\big(q_pc,v\big)_{\bar{m}}=(q_Ic_I,v)_{\bar{m}}, && \forall v\in S_h, && \text{(3.5a)}\\
&(\bar{z}^x,w^x)_x+(\bar{z}^y,w^y)_y+(\bar{z}^z,w^z)_z-(c,D_xw^x+D_xw^y+D_xw^z)_{\bar{m}}=0, && \forall \mathbf{w}\in V_h, && \text{(3.5b)}\\
&(z^x,w^x)_x+(z^y,w^y)_y+(z^z,w^z)_z\\
&\quad=(d_x(\mathbf{u})\bar{z}^x,w^x)_x+\big(d_y(\mathbf{u})\bar{z}^y,w^y\big)_y+(d_z(\mathbf{u})\bar{z}^z,w^z)_z, && \forall \mathbf{w}\in V_h. && \text{(3.5c)}
\end{aligned}$$

The UBCD scheme is defined for (3.3),

$$\begin{aligned}
&\Big(\phi\frac{C^n-C^{n-1}}{\Delta t_c},v\Big)_{\bar{m}}+(\nabla\cdot\mathbf{G},v)_{\bar{m}}+\big(D_xZ^{x,n}+D_yZ^{y,z}+D_zZ^{z,n},v\big)_{\bar{m}}-\big(q_pC^n,v\big)_{\bar{m}}\\
&\quad=(q_IC_I^n,v)_{\bar{m}}, && \forall v\in S_h, && \text{(3.6a)}\\
&(\bar{Z}^{x,n},w^x)_x+(\bar{Z}^{y,n},w^y)_y+(\bar{Z}^{z,n},w^z)_z-(C^n,D_xw^x+D_xw^y+D_xw^z)_{\bar{m}}=0, && \forall \mathbf{w}\in V_h, && \text{(3.6b)}\\
&(Z^{x,n},w^x)_x+(Z^{y,n},w^y)_y+(Z^{z,n},w^z)_z\\
&\quad=(d_x(E\mathbf{U}^n)\bar{Z}^{x,n},w^x)_x+\big(d_y(E\mathbf{U}^n)\bar{Z}^{y,n},w^y\big)_y+(d_z(E\mathbf{U}^n)\bar{Z}^{z,n},w^z)_z, && \forall \mathbf{w}\in V_h. && \text{(3.6c)}
\end{aligned}$$

Let $\bar{C}_m$ replace $c(t_m)$ in computing the nonlinear function $a(c)$, where C_m is the approximation of c_m,

$$\bar{C}_m=\min\{1,\max(0,C_m)\}\in[0,1]. \tag{3.7}$$

The value at t^n, $t_{m-1}<t^n\le t_m$, is assigned by a linear extrapolation

$$E\mathbf{U}^n=\begin{cases}\mathbf{U}_0, & t_0<t^n\le t_1, \quad m=1,\\ \Big(1+\dfrac{t^n-t_{m-1}}{t_{m-1}-t_{m-2}}\Big)\mathbf{U}_{m-1}-\dfrac{t^n-t_{m-1}}{t_{m-1}-t_{m-2}}\mathbf{U}_{m-2}, & t_{m-1}<t^n\le t_m, \quad m\ge 2.\end{cases} \tag{3.8}$$

Initial approximations:

$$C^0=\tilde{C}^0, \quad X\in\Omega, \tag{3.9}$$

where $\tilde{C}^0$ is the elliptic-projection or L^2-projection of c_0 (see the details in the following section).

The convection term of (3.6a) is treated by a simple upwind approximation where the approximation C is used. Since $\mathbf{g}=\mathbf{u}c=0$ on $\partial\Omega$, we assign the mean value of the integral of $\mathbf{G}^n\cdot\gamma$ by 0. σ is the interface of e_1 and e_2, X_l is the barycenter and γ_l is the unit normal vector to e_2. Let

$$\mathbf{G}^n\cdot\gamma=\begin{cases}C^n_{e_1}(E\mathbf{U}^n\cdot\gamma_l)(X_l), & (E\mathbf{U}^n\cdot\gamma_l)(X_l)\ge 0,\\ C^n_{e_2}(E\mathbf{U}^n\cdot\gamma_l)(X_l), & (E\mathbf{U}^n\cdot\gamma_l)(X_l)<0.\end{cases} \tag{3.10}$$

$C^n_{e_1}$ and $C^n_{e_2}$ are the constant values of C^n on e_1 and e_2, respectively. Then $\mathbf{G}^n$ is computed and the scheme of (3.6) is constructed. A nonsymmetric matrix is given to compute C. If $\mathbf{G}^n$ is defined by the values at the previous time level, then a symmetric matrix is formed

$$\mathbf{G}^n\cdot\gamma=\begin{cases}C^{n-1}_{e_1}(E\mathbf{U}^n\cdot\gamma_l)(x_l), & (E\mathbf{U}^n\cdot\gamma_l)(x_l)\ge 0,\\ C^{n-1}_{e_2}(E\mathbf{U}^n\cdot\gamma_l)(x_l), & (E\mathbf{U}^n\cdot\gamma_l)(x_l)<0.\end{cases} \tag{3.11}$$

The computational accuracy of saturations should be improved and the computational work is the largest. An upwind fractional step difference scheme is used for solving (1.6). Since bound water exists everywhere in numerical simulation of oil reservoir [7–10], we suppose that $c(X,t)\ge c_*>0$ for a positive constant c_*. The coefficients of (1.6) are positive definite

$$0<\bar{D}_*\le\hat{D}(c)\le\bar{D}^*, \quad 0<\bar{\phi}_*\le\phi c\le\bar{\phi}^*, \tag{3.12}$$

where $\hat{D}(c)=\phi c\kappa$ and $\bar{D}_*$, $\bar{D}^*$, $\bar{\phi}_*$, $\bar{\phi}^*$ are positive constants.

The UFSD scheme is defined as follows for (1.6),

$$\begin{aligned}\phi_{ijk}C^n_{ijk}\frac{S^{n-2/3}_{\alpha,ijk}-S^{n-1}_{\alpha,ijk}}{\Delta t_c}=&\delta_{\bar{x}}(\phi C^n\kappa_\alpha\delta_x S^{n-2/3}_\alpha)_{ijk}+\delta_{\bar{y}}(\phi C^n\kappa_\alpha\delta_y S^{n-1}_\alpha)_{ijk}\\ &+\delta_{\bar{z}}(\phi C^n\kappa_\alpha\delta_z S^{n-1}_\alpha)_{ijk}+Q_\alpha(C^n_{ijk},S^{n-1}_{\alpha,ijk}), \quad 1\le i\le M_1-1, \end{aligned}\tag{3.13a}$$

$$S^{n-2/3}_{\alpha,ijk}=h^n_{\alpha,ijk}, \qquad X_{ijk}\in\partial\Omega_h, \tag{3.13b}$$

and

$$\phi_{ijk}C^n_{ijk}\frac{S^{n-1/3}_{\alpha,ijk}-S^{n-2/3}_{\alpha,ijk}}{\Delta t_c}=\delta_{\bar{y}}(\phi C^n\kappa_\alpha\delta_y(S^{n-1/3}_\alpha-S^{n-1}_\alpha))_{ijk}, \qquad 1\le j\le M_2-1, \tag{3.14a}$$

$$S^{n-1/3}_{\alpha,ijk}=h^n_{\alpha,ijk}, \qquad X_{ijk}\in\partial\Omega_h, \tag{3.14b}$$

and

$$\phi_{ijk}C^n_{ijk}\frac{S^n_{\alpha,ijk}-S^{n-1/3}_{\alpha,ijk}}{\Delta t_c}=\delta_{\bar{z}}(\phi C^n\kappa_\alpha\delta_z(S^n_\alpha-S^{n-1}_\alpha))_{ijk}$$
$$-\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S^n_{\alpha,ijk},\qquad 1\le k\le M_3-1, \tag{3.15a}$$
$$S^n_{\alpha,ijk}=h^n_{\alpha,ijk},\qquad X_{ijk}\in\partial\Omega_h, \tag{3.15b}$$

where $\alpha=1,2,\cdots,n_c$,

$$\delta_{E\mathbf{U}^n,r}S^n_{\alpha,ijk}=(E\mathbf{U}^n)_{r,ijk}\{H(E\mathbf{U}^n_{r,ijk})\delta_{\bar{r}}+(1-H(E\mathbf{U}^n_{r,ijk}))\delta_r\}S^n_{\alpha,ijk},\quad r=x,y,z,$$
$$H(z)=\begin{cases}1, & z\ge 0,\\ 0, & z<0.\end{cases}$$

Initial approximations:

$$S^0_{\alpha,ijk}=s_{\alpha,0}(X_{ijk}),\quad X_{ijk}\in\bar{\Omega}_h,\quad \alpha=1,2,\cdots,n_c. \tag{3.16}$$

The composite procedures run as follows. First, (3.9) and (3.4) are combined to determine $\{\mathbf{U}_0,P_0\}$. Then, $\{C^1,\mathbf{Z}^1,\bar{\mathbf{Z}}^1\}$ is computed by using (3.6). Next, using the UFSD scheme of (3.13)-(3.15) and using the algorithm of speedup we get $\{S^{1/3}_\alpha\},S^{2/3}_\alpha\}$, then obtain $\{S^1_\alpha\}$, $\alpha=1,2,\cdots,n_c$, the numerical solutions of saturations at $t=t^1$. Then, numerical solutions at $t=t^1$ are obtained. In a similar procession, we obtain $\{C^2,\mathbf{Z}^2,\bar{\mathbf{Z}}^2\}$, $\{S^2_\alpha,\alpha=1,2,\cdots,n_c\}$, $\cdots$, $\{C^{j_0^*},\mathbf{Z}^{j_0^*},\bar{\mathbf{Z}}^{j_0^*}\}$, $\{S^{j_0^*}_\alpha,\alpha=1,2,\cdots,n_c\}$. For $m\ge 1$, let

$$C_m=C^{j_0^*+(m-1)j^*},$$

then apply (3.4a) and (3.4b) to get $\{\mathbf{U}_m,P_m\}$. Then from (3.6a)-(3.6c) and (3.13)-(3.15), we can obtain the numerical solutions:

$$\{C^{j_0^*+(m-1)j^*+1},\mathbf{Z}^{j_0^*+(m-1)j^*+1},\bar{\mathbf{Z}}^{j_0^*+(m-1)j^*+1}\},\quad \{S^{j_0^*+(m-1)j^*+1}_\alpha,\alpha=1,2,\cdots,n_c\},\cdots.$$

Repeat the computations to obtain all the numerical solutions. By positive definite condition (C), the solutions exist and are unique.

3.2 The local conservation of mass

Suppose that the problem of (1.1)-(1.5) has no source or sink, i.e., $q\equiv 0$, and suppose that the boundary is impermeable. On an element

$$e=\Omega_{ijk}=[x_{i-1/2},x_{i+1/2}]\times[y_{j-1/2},y_{j+1/2}]\times[z_{k-1/2},z_{k+1/2}],$$

the local conservation of mass is addressed for the concentration

$$\int_e\phi\frac{\partial c}{\partial t}dX-\int_{\partial e}\mathbf{g}\cdot\gamma_e dS-\int_{\partial e}\mathbf{z}\cdot\gamma_e dS=0. \tag{3.17}$$

∂e is the boundary of e and γ_e is the outer normal vector. The discrete formula of local conservation is given in the following theorem.

Theorem 3.1. *If $q\equiv 0$, then on every element $e\in\Omega$,* (3.6a) *has the conservation of mass*

$$\int_e \phi\frac{C^n-C^{n-1}}{\Delta t_c}dX-\int_{\partial e}\mathbf{G}^n\cdot\gamma_e dS-\int_{\partial e}\mathbf{Z}^n\cdot\gamma_e dS=0. \tag{3.18}$$

Proof. For $v\in S_h$, let

$$v=\begin{cases} 1 & \text{on } e=\Omega_{ijk},\\ 0, & \text{otherwise,}\end{cases}$$

then reformulate (3.6a) as

$$\Big(\phi\frac{C^n-C^{n-1}}{\Delta t_c},1\Big)_{\Omega_{ijk}}-\int_{\partial e}\mathbf{G}^n\cdot\gamma_e dS+\big(D_xZ^{x,n}+D_yZ^{y,n}+D_zZ^{z,n},1\big)_{\Omega_{ijk}}=0. \tag{3.19}$$

Using the notation in Section 2, we have

$$\Big(\phi\frac{C^n-C^{n-1}}{\Delta t_c},1\Big)_{\Omega_{ijk}}=\phi_{ijk}\Big(\frac{C^n_{ijk}-C^{n-1}_{ijk}}{\Delta t_c}\Big)h_{x_i}h_{y_j}h_{z_k}=\int_{\Omega_{ijk}}\phi\frac{C^n-C^{n-1}}{\Delta t_c}dX, \tag{3.20a}$$

$$\begin{aligned}&\big(D_xZ^{x,n}+D_yZ^{y,n}+D_zZ^{z,n},1\big)_{\Omega_{ijk}}\\ &=\Big(Z^{x,n}_{i+1/2,jk}-Z^{x,n}_{i-1/2,jk}\Big)h_{y_j}h_{z_k}+\Big(Z^{y,n}_{i,j+1/2,k}-Z^{y,n}_{i,j-1/2,k}\Big)h_{x_i}h_{z_k}\\ &\quad+\Big(Z^{z,n}_{ij,k+1/2}-Z^{z,n}_{ij,k-1/2}\Big)h_{x_i}h_{y_j}=-\int_{\partial\Omega_{ijk}}\mathbf{Z}^n\cdot\gamma_{\partial\Omega_{ijk}}dS.\end{aligned} \tag{3.20b}$$

Substituting (3.20) into (3.19), we complete the proof. □

Then the whole conservation of mass is concluded.

Theorem 3.2. *Under the assumptions that $q\equiv 0$ and the boundary is impermeable,* (3.6a) *has the conservation on the whole domain*

$$\int_\Omega \phi\frac{C^n-C^{n-1}}{\Delta t_c}dX=0,\quad n>0. \tag{3.21}$$

Proof. Summing (3.18) on all the elements, we have

$$\sum_e\int_e \phi\frac{C^n-C^{n-1}}{\Delta t_c}dX-\sum_e\int_{\partial e}\mathbf{G}^n\cdot\gamma_e dS-\sum_e\int_{\partial e}\mathbf{Z}^n\cdot\gamma_e dS=0. \tag{3.22}$$

σ_l denotes the interface of e_1 and e_2, X_l is the barycenter, and γ_l is the outer normal vector to e_2. Recalling the definition of the diffusion, we can see that if

$$E\mathbf{U}^n\cdot\gamma_l(X)\geq 0\quad \text{on}\quad e_1,$$

then

$$\int_{\sigma_l}\mathbf{G}^n\cdot\gamma_l ds=C^n_{e_1}E\mathbf{U}^n\cdot\gamma_l(X)|\sigma_l|. \tag{3.23a}$$

Here $|\sigma_l|$ denotes the measure of σ_l. The outer normal vector on e_2 is $-\gamma_l$, so

$$E\mathbf{U}^n\cdot(-\gamma_l(X))\leq 0.$$

Then,

$$\int_{\sigma_l}\mathbf{G}^n\cdot(-\gamma_l)ds=-C^n_{e_1}E\mathbf{U}^n\cdot\gamma_l(X)|\sigma_l|. \tag{3.23b}$$

Since (3.23b) is opposite to (3.23a), so we have

$$\sum_e\int_{\partial e}\mathbf{G}^n\cdot\gamma_e dS=0. \tag{3.24}$$

Combining the following fact

$$-\sum_e\int_{\partial e}\mathbf{Z}^n\cdot\gamma_e dS=-\int_{\partial\Omega}\mathbf{Z}^n\cdot\gamma_\Omega dS=0, \tag{3.25}$$

and substituting (3.24), (3.25) into (3.22), we have

$$\int_\Omega\phi\frac{C^n-C^{n-1}}{\Delta t_c}dX=0,\quad n>0. \tag{3.26}$$

The proof is completed. The conservation of mass is important in numerical simulation of seepage mechanics. □

4 Convergence analysis

First we introduce an auxiliary elliptic-projection. Define $\tilde{\mathbf{U}}\in V_h$, $\tilde{P}\in S_h$ by

$$\big(D_x\tilde{U}^x+D_y\tilde{U}^y+D_z\tilde{U}^z,v\big)_{\bar{m}}=(q,v)_{\bar{m}},\qquad\forall v\in S_h, \tag{4.1a}$$

$$\begin{aligned}&\Big(a^{-1}(c)\tilde{U}^x,w^x\Big)_x+\Big(a^{-1}(c)\tilde{U}^y,w^y\Big)_y+\Big(a^{-1}(c)\tilde{U}^z,w^z\Big)_z\\&\quad-\big(\tilde{P},D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}}=0,\qquad\forall\mathbf{w}\in V_h,\end{aligned} \tag{4.1b}$$

where c is the exact solution of (1.1) and (1.2a).

Let

$$F=q_pc+q_Ic_I-\Big(\psi\frac{\partial c}{\partial t}+\nabla\cdot\mathbf{g}\Big).$$

Define $\tilde{\mathbf{Z}},\tilde{\tilde{\mathbf{Z}}}\in V_h$ and $\tilde{C}\in S_h$ by

$$\big(D_x\tilde{Z}^x+D_y\tilde{Z}^y+D_z\tilde{Z}^z,v\big)_{\bar{m}}=(F,v)_{\bar{m}},\qquad\forall v\in S_h, \tag{4.2a}$$

$$\Big(\tilde{\tilde{\mathbf{Z}}}^x,w^x\Big)_x+\Big(\tilde{\tilde{\mathbf{Z}}}^y,w^y\Big)_y+\Big(\tilde{\tilde{\mathbf{Z}}}^z,w^z\Big)_z=\big(\tilde{C},D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}},\qquad\forall\mathbf{w}\in V_h, \tag{4.2b}$$

$$\begin{aligned}\big(\tilde{\mathbf{Z}}^x,w^x\big)_x+\big(\tilde{\mathbf{Z}}^y,w^y\big)_y+\big(\tilde{\mathbf{Z}}^z,w^z\big)_z=&\Big(d_x(\mathbf{u})\tilde{\tilde{\mathbf{Z}}}^x,w^x\Big)_x+\Big(d_y(\mathbf{u})\tilde{\tilde{\mathbf{Z}}}^y,w^y\Big)_y\\&+\Big(d_z(\mathbf{u})\tilde{\tilde{\mathbf{Z}}}^z,w^z\Big)_z,\qquad\forall\mathbf{w}\in V_h.\end{aligned} \tag{4.2c}$$

Let $\pi=P-\tilde{P}$, $\eta=\tilde{P}-p$, $\boldsymbol{\sigma}=\mathbf{U}-\tilde{\mathbf{U}}$, $\boldsymbol{\rho}=\tilde{\mathbf{U}}-\mathbf{u}$, $\xi_c=C-\tilde{C}$, $\zeta_c=\tilde{C}-c$, $\alpha_z=\mathbf{Z}-\tilde{\mathbf{Z}}$, $\beta_z=\tilde{\mathbf{Z}}-\mathbf{z}$, $\bar{\alpha}_z=\bar{\mathbf{Z}}-\tilde{\bar{\mathbf{Z}}}$, $\bar{\beta}_z=\tilde{\bar{\mathbf{Z}}}-\bar{\mathbf{z}}$. Suppose that (1.1)-(1.5) is positive definite (C), and the exact solutions satisfy regularity (R). From the theory of Weiser and Wheeler [22] and the discussion of Arbogast, Wheeler and Yotov [45], it is easy to see that the auxiliary functions $\{\tilde{P},\tilde{\mathbf{U}},\tilde{C},\tilde{\mathbf{Z}},\tilde{\bar{\mathbf{Z}}}\}$ of (4.1) and (4.2) exist and are unique.

Lemma 4.1. *The coefficients and exact solutions of* (1.1)-(1.5) *are supposed to satisfy* (C) *and* (R). *Then, there exist two positive constants $\bar{C}_1$ and $\bar{C}_2$ independent of h and Δt, such that*

$$||\eta||_{\bar{m}}+||\zeta_c||_{\bar{m}}+|||\mathbf{fi}_z|||+|||\bar{\mathbf{fi}}_z|||+\left|\left|\frac{\partial\zeta_c}{\partial t}\right|\right|_{\bar{m}}\le\bar{C}_1\{h_p^2+h_c^2\}, \tag{4.3a}$$

$$|||\tilde{\mathbf{U}}|||_\infty+|||\tilde{\mathbf{Z}}|||_\infty+\left|\left|\left|\tilde{\bar{\mathbf{Z}}}\right|\right|\right|_\infty\le C_2. \tag{4.3b}$$

We estimate π and σ first. Subtracting (4.1a) ($t=t_m$) and (4.1b) ($t=t_m$), respectively, from (3.4a) and (3.4b), we obtain

$$\begin{aligned}&\big(D_x\sigma_m^x+D_y\sigma_m^y+D_z\sigma_m^z,v\big)_{\bar{m}}=0, && \forall v\in S_h, && (4.4a)\\&\Big(a^{-1}(\bar{C}_m^x)\sigma_m^x,w^x\Big)_x+\Big(a^{-1}(\bar{C}_m^y)\sigma_m^y,w^y\Big)_y+\Big(a^{-1}(\bar{C}_m^z)\sigma_m^z,w^z\Big)_z\\&\quad-\big(\pi_m,D_xw^x+D_yw^y+D_zw^z\big)_{\bar{m}}\\&=-\sum_{r=x,y,z}\Big(\big(a^{-1}(\bar{C}_m^r)-a^{-1}(c_m)\big)\tilde{U}_m^r,w^r\Big)_r, && \forall \mathbf{w}\in V_h. && (4.4b)\end{aligned}$$

Taking $v=\pi_m$ in (4.4a) and $w=\sigma_m$ in (4.4b) to get

$$\begin{aligned}&\Big(a^{-1}(\bar{C}_m^x)\sigma_m^x,\sigma_m^x\Big)_x+\Big(a^{-1}(\bar{C}_m^y)\sigma_m^y,\sigma_m^y\Big)_y+\Big(a^{-1}(\bar{C}_m^z)\sigma_m^z,\sigma_m^z\Big)_z\\=&-\sum_{r=x,y,z}\Big((a^{-1}(\bar{C}_m^r)-a^{-1}(c_m))\tilde{U}_m^r,\sigma_m^r\Big)_r.\end{aligned} \tag{4.5}$$

Using (4.5), Lemma 2.1-Lemma 4.1, the Taylor's formula and the positive definiteness (C), we have

$$\begin{aligned}|||\sigma_m|||^2\le&K\sum_{r=x,y,z}||\bar{C}_m^r-c_m||_{\bar{m}}^2\\\le&K\Big\{\sum_{r=x,y,z}||\bar{c}_m^r-c_m||_{\bar{m}}^2+||\xi_{c,m}||_{\bar{m}}^2+||\zeta_{c,m}||_{\bar{m}}^2+(\Delta t_c)^2\Big\}\\\le&K\Big\{||\xi_{c,m}||_{\bar{m}}^2+h_c^4+(\Delta t_c)^2\Big\}.\end{aligned} \tag{4.6}$$

A duality method is used to estimate $\pi_m\in S_h$ [46, 47]. Consider the following elliptic problem,

$$\begin{aligned}&\nabla\cdot\omega=\pi_m, && X=(x,y,z)^T\in\Omega, && (4.7a)\\&\omega=\nabla p, && X\in\Omega, && (4.7b)\\&\omega\cdot\gamma=0, && X\in\partial\Omega. && (4.7c)\end{aligned}$$

It follows from the regularity that

$$\sum_{r=x,y,z}\left|\left|\frac{\partial\omega^r}{\partial r}\right|\right|_{\bar{m}}^2\leq K||\pi_m||_{\bar{m}}^2. \tag{4.8}$$

Consider the following equation

$$\left(\frac{\partial\tilde{\omega}^r}{\partial r},v\right)_{\bar{m}}=\left(\frac{\partial\omega^r}{\partial r},v\right)_{\bar{m}},\quad \forall v\in S_h,\quad r=x,y,z. \tag{4.9a}$$

The solution $\tilde{\omega}$ exists and satisfies

$$\sum_{r=x,y,z}\left|\left|\frac{\partial\tilde{\omega}^r}{\partial r}\right|\right|_{\bar{m}}^2\leq\sum_{r=x,y,z}\left|\left|\frac{\partial\omega^r}{\partial r}\right|\right|_{\bar{m}}^2. \tag{4.9b}$$

By Lemma 2.4, (4.7), (4.8) and (4.6), we have

$$\begin{aligned}||\pi_m||_{\bar{m}}^2&=(\pi_m,\nabla\cdot\omega)=\left(\pi_m,D_x\tilde{\omega}^x+D_y\tilde{\omega}^y+D_z\tilde{\omega}^z\right)_{\bar{m}}\\&=\sum_{r=x,y,z}\left(a^{-1}(\bar{C}_m^r)\sigma_m^r,\tilde{\omega}^r\right)_r+\sum_{r=x,y,z}\left((a^{-1}(\bar{C}_m^r)-a^{-1}(c_m))\tilde{U}_m^r,\tilde{\omega}^r\right)_r\\&\leq K|||\tilde{\omega}|||\left\{|||\sigma_m|||^2+||\xi_{c,m}||_{\bar{m}}^2+h_c^4+(\Delta t_c)^2\right\}^{1/2}.\end{aligned} \tag{4.10}$$

Using Lemma 2.4, (4.8) and (4.9a), we obtain

$$\begin{aligned}|||\tilde{\omega}|||^2&\leq\sum_{r=x,y,z}||D_r\tilde{\omega}^r||_{\bar{m}}^2\\&=\sum_{r=x,y,z}\left|\left|\frac{\partial\tilde{\omega}^r}{\partial r}\right|\right|_{\bar{m}}^2\leq\sum_{r=x,y,z}\left|\left|\frac{\partial\omega^r}{\partial r}\right|\right|_{\bar{m}}^2\\&\leq K||\pi_m||_{\bar{m}}^2.\end{aligned} \tag{4.11}$$

Substituting (4.11) into (4.10) gives

$$||\pi_m||_{\bar{m}}^2\leq K\left\{|||\sigma_m|||^2+||\xi_{c,m}||_{\bar{m}}^2+h_c^4+(\Delta t_c)^2\right\}\leq K\left\{||\xi_{c,m}||_{\bar{m}}^2+h_c^4+(\Delta t_c)^2\right\}. \tag{4.12}$$

The upwind term is discussed later. Some symbols are introduced. σ denotes a surface of e, and γ_l is the unit outer normal vector. (σ,γ_l) determines two adjacent elements e^+ and e^-, where they have a common surface and γ_l is defined towards e^+. For $f\in S_h$ and $x\in\sigma$, define

$$f^-(x)=\lim_{s\to 0-}f(x+s\gamma_l),\quad f^+(x)=\lim_{s\to 0+}f(x+s\gamma_l),$$

and let $[f]=f^+-f^-$.

Lemma 4.2. *For $f_1,f_2\in S_h$, we have*

$$\int_\Omega \nabla\cdot(\mathbf{u}f_1)f_2dx=\frac{1}{2}\sum_\sigma\int_\sigma [f_1][f_2]|\mathbf{u}\cdot\gamma|ds+\frac{1}{2}\sum_\sigma\int_\sigma \mathbf{u}\cdot\gamma_l(f_1^++f_1^-)(f_2^--f_2^+)ds. \tag{4.13}$$

Proof. Note that

$$\begin{aligned}&\int_\Omega \nabla\cdot(\mathbf{u}f_1)f_2dx=\sum_e\int_{\Omega_e}\nabla\cdot(\mathbf{u}f_1)f_2dx\\ =&\sum_\sigma\int_\sigma\big[(\mathbf{u}\cdot\gamma_l)_+f_1^{e^-}f_2^{e^-}+(\mathbf{u}\cdot\gamma_l)_-f_1^{e^+}f_2^{e^-}+(\mathbf{u}\cdot(-\gamma_l))_+f_1^{e^+}f_2^{e^+}+(\mathbf{u}\cdot(-\gamma_l))_-f_1^{e^-}f_2^{e^+}\big]ds,\end{aligned}$$

where

$$(\mathbf{u}\cdot\gamma)_+=\max\{\mathbf{u}\cdot\gamma,0\}\quad\text{and}\quad(\mathbf{u}\cdot\gamma)_-=\min\{\mathbf{u}\cdot\gamma,0\}.$$

Using the equalities

$$\begin{aligned}&(\mathbf{u}\cdot(-\gamma_l))_+=-(\mathbf{u}\cdot\gamma_l)_-, && (\mathbf{u}\cdot(-\gamma_l))_-=-(\mathbf{u}\cdot\gamma_l)_+,\\ &f^{e^+}=f^r, && f^{e^-}=f^l,\end{aligned}$$

we have

$$\begin{aligned}&\int_\Omega \nabla\cdot(\mathbf{u}f_1)f_2dx=\sum_\sigma\int_\sigma\big[(\mathbf{u}\cdot\gamma_l)_+f_1^l(f_2^l-f_2^r)+(\mathbf{u}\cdot\gamma_l)_-f_1^r(f_2^l-f_2^r)\big]ds\\ =&\sum_\sigma\int_\sigma\big[((\mathbf{u}\cdot\gamma_l)_+-(\mathbf{u}\cdot\gamma_l)_-)f_1^l(f_2^l-f_2^r)+(\mathbf{u}\cdot\gamma_l)_-(f_1^r+f_1^l)(f_2^l-f_2^r)\big]ds\\ =&\sum_\sigma\int_\sigma\big[|\mathbf{u}\cdot\gamma_l|(f_1^l-f_1^r)(f_2^l-f_2^r)+|\mathbf{u}\cdot\gamma_l|f_1^r(f_2^l-f_2^r)+(\mathbf{u}\cdot\gamma_l)_-(f_1^r+f_1^l)(f_2^l-f_2^r)\big]ds\\ =&\sum_\sigma\int_\sigma\Big[\frac{1}{2}|\mathbf{u}\cdot\gamma_l|(f_1^l-f_1^r)(f_2^l-f_2^r)+(f_2^l-f_2^r)\Big(\frac{1}{2}|\mathbf{u}\cdot\gamma_l|(f_1^l-f_1^r)+|\mathbf{u}\cdot\gamma_l|f_1^r\\ &\quad+(\mathbf{u}\cdot\gamma_l)_-(f_1^r+f_1^l)\Big)\Big]ds\\ =&\sum_\sigma\int_\sigma\Big[\frac{1}{2}|\mathbf{u}\cdot\gamma_l|(f_1^l-f_1^r)(f_2^l-f_2^r)+(f_2^l-f_2^r)\Big(\frac{1}{2}|\mathbf{u}\cdot\gamma_l|(f_1^l+f_1^r)+(\mathbf{u}\cdot\gamma_l)_-(f_1^r+f_1^l)\Big)\Big]ds\\ =&\sum_\sigma\int_\sigma\Big[\frac{1}{2}|\mathbf{u}\cdot\gamma_l|(f_1^l-f_1^r)(f_2^l-f_2^r)+(\mathbf{u}\cdot\gamma_l)\frac{1}{2}(f_1^l+f_1^r)(f_2^l-f_2^r)\Big]ds,\end{aligned}$$

where $f^r=f^+$, $f^l=f^-$. Then, the proof is completed. □

The concentration equation (1.2a) is considered now. Subtracting (4.2) at $t=t^n$ from (3.6), we have

$$\begin{aligned}&\Big(\phi\frac{C^n-C^{n-1}}{\Delta t_c},v\Big)_{\bar m}+\big(\nabla\cdot\mathbf{G}^n,v\big)_{\bar m}+\Big(\sum_{r=x,y,z}D_r\alpha_z^{r,n},v\Big)_{\bar m}\\ &=\Big(q_p(\xi_c^n+\zeta_c^n)+\phi\frac{\partial c^n}{\partial t}+\nabla\cdot\mathbf{g}^n,v\Big)_{\bar m},\qquad\forall v\in S_h,\end{aligned} \tag{4.14a}$$

$$\left(\bar{\alpha}_z^{x,n},w^x\right)_x+\left(\bar{\alpha}_z^{y,n},w^y\right)_y+\left(\bar{\alpha}_z^{z,n},w^z\right)_z=\Big(\xi_c^n,\sum_{r=x,y,z}D_r w^r\Big)_{\bar{m}},\qquad \forall \mathbf{w}\in V_h, \tag{4.14b}$$

$$\begin{aligned}&\left(\alpha_z^{x,n},w^x\right)_x+\left(\alpha_z^{y,n},w^y\right)_y+\left(\alpha_z^{z,n},w^z\right)_z\\ &=\Big(d_x(E\mathbf{U}^n)\bar{Z}^{x,n}-d_x(\mathbf{u}^n)\bar{\bar{Z}}^{x,n},w_x\Big)_x+\Big(d_y(E\mathbf{U}^n)\bar{Z}^{y,n}-d_y(\mathbf{u}^n)\bar{\bar{Z}}^{y,n},w_y\Big)_y\\ &\quad+\Big(d_z(E\mathbf{U}^n)\bar{Z}^{z,n}-d_z(\mathbf{u}^n)\bar{\bar{Z}}^{z,n},w_z\Big)_z,\qquad \forall \mathbf{w}\in V_h.\end{aligned} \tag{4.14c}$$

Taking $v=\xi_c^n$ in (4.14a), $\mathbf{w}=\alpha_z^n$ in (4.14b) and $\mathbf{w}=\bar{\alpha}_z^n$ in (4.14c), then subtracting (4.14c) from the sum of (4.14a) and (4.14b), we have

$$\begin{aligned}&\Big(\phi\frac{\xi_c^n-\xi_c^{n-1}}{\Delta t_c},\xi_c^n\Big)_{\bar{m}}+\Big(\nabla\cdot(\mathbf{G}^n-\mathbf{g}^n),\xi_c^n\Big)_{\bar{m}}\\ =&\left(q_p\xi_c^n,\xi_c^n\right)_{\bar{m}}+\Big(q_p\zeta_c^n-\phi\frac{\zeta_c^n-\zeta_c^{n-1}}{\Delta t_c},\xi_c^n\Big)_{\bar{m}}+\Big(\phi\Big(\frac{\partial c^n}{\partial t}-\frac{c^n-c^{n-1}}{\Delta t_c}\Big),\xi_c^n\Big)_{\bar{m}}\\ &-\sum_{r=x,y,z}\Big(d_r(E\mathbf{U}^n)\bar{\alpha}_z^{r,n},\bar{\alpha}_z^{r,n}\Big)_r+\sum_{r=x,y,z}\Big([d_r(\mathbf{u}^n)-d_r(E\mathbf{U}^n)]\bar{\bar{Z}}^{r,n},\bar{\alpha}_z^{r,n}\Big)_r.\end{aligned} \tag{4.15}$$

Continue,

$$\begin{aligned}&\Big(\phi\frac{\xi_c^n-\xi_c^{n-1}}{\Delta t_c},\xi_c^n\Big)_{\bar{m}}+\sum_{r=x,y,z}\Big(d_r(E\mathbf{U}^n)\bar{\alpha}_z^{r,n},\bar{\alpha}_z^{r,n}\Big)_r+\Big(\nabla\cdot(\mathbf{G}^n-\mathbf{g}^n),\xi_c^n\Big)_{\bar{m}}\\ =&\left(q_p\xi_c^n,\xi_c^n\right)_{\bar{m}}+\Big(q_p\zeta_c^n-\phi\frac{\zeta_c^n-\zeta_c^{n-1}}{\Delta t_c},\xi_c^n\Big)_{\bar{m}}+\Big(\phi\Big(\frac{\partial c^n}{\partial t}-\frac{c^n-c^{n-1}}{\Delta t_c}\Big),\xi_c^n\Big)_{\bar{m}}\\ &+\sum_{r=x,y,z}\Big([d_r(\mathbf{u}^n)-d_r(E\mathbf{U}^n)]\bar{\bar{Z}}^{r,n},\bar{\alpha}_z^{r,n}\Big)_r\\ =&T_1+T_2+T_3+T_4.\end{aligned} \tag{4.16}$$

The terms on the left-hand side of (4.16) are estimated as follows,

$$\Big(\phi\frac{\xi_c^n-\xi_c^{n-1}}{\Delta t_c},\xi_c^n\Big)_{\bar{m}}\geq\frac{1}{2\Delta t_c}\Big\{\left(\phi\xi_c^n,\xi_c^n\right)_{\bar{m}}-\Big(\phi\xi_c^{n-1},\xi_c^{n-1}\Big)_{\bar{m}}\Big\}, \tag{4.17a}$$

$$\sum_{r=x,y,z}\Big(d_r(E\mathbf{U}^n)\bar{\alpha}_z^{r,n},\bar{\alpha}_z^{r,n}\Big)_r\geq D_*\big|\big|\big|\bar{\alpha}_z^n\big|\big|\big|^2. \tag{4.17b}$$

The third term is divided into

$$\left(\nabla\cdot(\mathbf{G}^n-\mathbf{g}^n),\xi_c^n\right)_{\bar{m}}=\left(\nabla\cdot(\mathbf{G}^n-\Pi\mathbf{g}^n),\xi_c^n\right)_{\bar{m}}+\left(\nabla\cdot(\Pi\mathbf{g}^n-\mathbf{g}^n),\xi_c^n\right)_{\bar{m}}. \tag{4.18}$$

$\Pi\mathbf{g}$ is defined similarly to $\mathbf{G}$,

$$\Pi\mathbf{g}^n\cdot\gamma_l=\begin{cases}\Pi c_{e_1}^n(E\mathbf{U}^n\cdot\gamma_l)(x_l), & (E\mathbf{U}^n\cdot\gamma_l)(x_l)\geq 0,\\ \Pi c_{e_2}^n(E\mathbf{U}^n\cdot\gamma_l)(x_l), & (E\mathbf{U}^n\cdot\gamma_l)(x_l)<0.\end{cases}$$

Using Lemma 4.2 and (4.13) to obtain

$$\begin{aligned}
&\big(\nabla\cdot(\mathbf{G}^n-\Pi\mathbf{g}^n),\xi_c^n\big)_{\bar{m}}=\sum_e\int_{\Omega_e}\nabla\cdot(\mathbf{G}^n-\Pi\mathbf{g}^n)\xi_c^n dx=\sum_e\int_{\Omega_e}\nabla\cdot(E\mathbf{U^n}\xi_c^n)\xi_c^n dx\\
&=\frac{1}{2}\sum_\sigma\int_\sigma|E\mathbf{U^n}\cdot\gamma_l|[\xi_c^n]^2ds-\frac{1}{2}\sum_\sigma\int_\sigma(E\mathbf{U^n}\cdot\gamma_l)(\xi_c^{n,+}+\xi_c^{n,-})[\xi_c^n]^2ds\\
&=Q_1+Q_2,\\
&Q_1=\frac{1}{2}\sum_\sigma\int_\sigma|E\mathbf{U^n}\cdot\gamma_l|[\xi_c^n]^2ds\geq 0,\\
&Q_2=-\frac{1}{2}\sum_\sigma\int_\sigma(E\mathbf{U^n}\cdot\gamma_l)[(\xi_c^{n,+})^2-(\xi_c^{n,-})^2]ds=\frac{1}{2}\sum_e\int_{\Omega_e}\nabla\cdot E\mathbf{U^n}(\xi_c^n)^2dx\\
&\quad=\frac{1}{2}\sum_e\int_{\Omega_e}q^n(\xi_c^n)^2dx.
\end{aligned}$$

Move Q_2 to the right-hand side of (4.16). Since $\mathbf{q}$ is bounded, we have

$$|Q_2|\leq K||\xi_c^n||_{\bar{m}}^2.$$

For the second term of (4.17c), we have

$$\begin{aligned}
&\big(\nabla\cdot(\mathbf{g}^n-\Pi\mathbf{g}^n),\xi_c^n\big)_{\bar{m}}=\sum_\sigma\int_\sigma\{c^n\mathbf{u}^n\cdot\gamma_l-\Pi c^nE\mathbf{U}^n\cdot\gamma_l\}[\xi_c^n]^2ds\\
=&\sum_\sigma\int_\sigma\{c^n\mathbf{u}^n-c^nE\mathbf{u}^n+c^nE\mathbf{u}^n-c^nE\mathbf{U}^n+c^nE\mathbf{U}^n-\Pi c^nE\mathbf{U}^n\}\cdot\gamma_l[\xi_c^n]^2ds\\
=&\big(\nabla\cdot(c^n\mathbf{u}^n-c^nE\mathbf{u}^n),\xi_c^n\big)_{\bar{m}}+\big(\nabla\cdot c^nE(\mathbf{u}^n-\mathbf{U}^n),\xi_c^n\big)_{\bar{m}}+\sum_\sigma\int_\sigma E\mathbf{U}^n\cdot\gamma_l(c^n-\Pi c^n)[\xi_c^n]ds\\
\leq&K\Big\{\Delta t_p^4+||E(\mathbf{u}^n-\mathbf{U}^n)||_{H(\mathrm{div})}^2+||\xi_c^n||_{\bar{m}}^2\Big\}+K\sum_\sigma\int_\sigma|E\mathbf{U}^n\cdot\gamma_l||c^n-\Pi c^n|^2ds\\
&+\frac{1}{4}\sum_\sigma\int_\sigma|E\mathbf{U}^n\cdot\gamma_l|[\xi_c^n]^2ds.
\end{aligned}$$

Using (4.6), (4.12), Lemma 4.1 and the discussion in [22,45], we have

$$|c^n-\Pi c^n|=\mathcal{O}(h_c^2),$$

then

$$\begin{aligned}
\big(\nabla\cdot(\mathbf{g}^n-\Pi\mathbf{g}^n),\xi_c^n\big)_{\bar{m}}\leq&K\Big\{\Delta t_p^4+h_p^4+h_c^2+||\xi_c^n||_{\bar{m}}^2+||\xi_{c,m-1}||_{\bar{m}}^2+||\xi_{c,m-2}||_{\bar{m}}^2\Big\}\\
&+\frac{1}{4}\sum_\sigma\int_\sigma|E\mathbf{U}^n\cdot\gamma_l|[\xi_c^n]^2ds. \qquad (4.19)
\end{aligned}$$

Consider the terms on the right-hand side of (4.16),

$$|T_1|+|T_2|+|T_3|\leq K\Delta t_c\Big\|\frac{\partial^2 c}{\partial t^2}\Big\|^2_{L^2(t^{n-1},t^n;\bar{m})}+K\{||\xi_c^n||^2_{\bar{m}}+h_c^4\}. \tag{4.20a}$$

T_4 is estimated by using (4.6), (4.12) and Lemma 4.1,

$$|T_4|\leq\varepsilon|||\bar{\alpha}_z^n|||^2+K\Big\{(\Delta t_p)^3\Big\|\frac{\partial \mathbf{u}}{\partial t}\Big\|^2_{L^2(t_{m-1},t_m;\bar{m})}+h_p^4+||\zeta_{c,m-1}||^2_{\bar{m}}+||\zeta_{c,m-2}||^2_{\bar{m}}\Big\}. \tag{4.20b}$$

Substituting (4.17) and (4.20) into (4.16), we have

$$\begin{aligned}&\frac{1}{2\Delta t_c}\Big\{||\phi^{1/2}\xi_c^n||^2_{\bar{m}}-||\phi^{1/2}\xi_c^{n-1}||^2_{\bar{m}}\Big\}+\frac{D_*}{2}|||\bar{\alpha}_z^n|||^2+\frac{1}{2}\sum_\sigma\int_\sigma|E\mathbf{U^n}\cdot\gamma_l|[\xi_c^n]^2ds\\ \leq& K\Big\{\Delta t_c\Big\|\frac{\partial^2 c}{\partial t^2}\Big\|^2_{L^2(t^{n-1},t^n;\bar{m})}+(\Delta t_p)^3\Big\|\frac{\partial \mathbf{u}}{\partial t}\Big\|^2_{L^2(t_{m-1},t_m;\bar{m})}+||\xi_c^n||^2_{\bar{m}}+||\zeta_{c,m-1}||^2_{\bar{m}}\\ &+||\zeta_{c,m-2}||^2_{\bar{m}}+h_c^2+h_p^4\Big\}+\frac{1}{4}\sum_\sigma\int_\sigma|E\mathbf{U}^n\cdot\gamma_l|[\xi_c^n]^2ds.\end{aligned} \tag{4.21}$$

Move the last term on the right-hand side to the left-hand side. Multiplying both sides by $2\Delta t_c$, summing them on n, and using $\xi_c^0=0$ and (3.8), we have

$$\begin{aligned}&||\phi^{1/2}\xi_c^N||^2_{\bar{m}}+\sum_{n=1}^N|||\bar{\alpha}_z^n|||^2\Delta t_c\\ \leq& K\Big\{h_p^4+h_c^2+(\Delta t_c)^2+(\Delta t_{p,1})^3+(\Delta t_p)^4\Big\}+K\sum_{n=1}^N||\xi_c^n||^2_{\bar{m}}\Delta t_c.\end{aligned} \tag{4.22}$$

Applying the discrete Gronwall lemma gives

$$||\xi_c^N||^2_{\bar{m}}+\sum_{n=0}^N|||\bar{\alpha}^n|||^2\Delta t_c\leq K\Big\{h_p^4+h_c^2+(\Delta t_c)^2+(\Delta t_{p,1})^3+(\Delta t_p)^4\Big\}. \tag{4.23}$$

It follows from (4.6), (4.12) and (4.23),

$$\sup_{0\leq m\leq M}\Big\{||\pi_m||^2_{\bar{m}}+|||\sigma_m|||^2\Big\}\leq K\Big\{h_p^4+h_c^2+(\Delta t_c)^2+(\Delta t_{p,1})^3+(\Delta t_p)^4\Big\}. \tag{4.24}$$

Next, the UFSD is argued. Let

$$\xi^n_{\alpha,ijk}=s_\alpha(X_{ijk},t^n)-S^n_{\alpha,ijk}.$$

Eliminating $S_\alpha^{n-2/3}$, $S_\alpha^{n-1/3}$ and writing a combination equation of (3.13)-(3.15) as follows,

$$\begin{aligned}&\phi_{ijk}C^n_{ijk}\frac{S^n_{\alpha,ijk}-S^{n-1}_{\alpha,ijk}}{\Delta t_c}-\sum_{r=x,y,z}\delta_{\bar{r}}(C^n\phi\kappa_\alpha\delta_r S^n_\alpha)_{ijk}\\ =&-\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S^n_{\alpha,ijk}+Q_\alpha(C^n_{ijk},S^{n-1}_{\alpha,ijk})-S^{n-1}_{\alpha,ijk}\Big(q^n_{ijk}+\phi\frac{C^n_{ijk}-C^{n-1}_{ijk}}{\Delta t_c}\Big)\end{aligned}$$

$$
\begin{aligned}
&-(\Delta t_c)^2\Big\{\delta_{\bar{x}}(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1}\delta_{\bar{y}}(C^n\phi\kappa_\alpha\delta_y(d_tS_\alpha^{n-1}))))_{ijk}+\cdots\\
&+\delta_{\bar{y}}(C^n\phi\kappa_\alpha\delta_y((C^n\phi)^{-1}\delta_{\bar{z}}(C^n\phi\kappa_\alpha\delta_z(d_tS_\alpha^{n-1}))))_{ijk}\Big\}\\
&+(\Delta t_c)^3\delta_{\bar{x}}(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1}\delta_{\bar{y}}(C^n\phi\kappa_\alpha\delta_y((C^n\phi)^{-1}\delta_{\bar{z}}(C^n\phi\kappa_\alpha\delta_z(d_tS_\alpha^{n-1}))))))_{ijk}\\
&-\Delta t_c\Big\{\delta_{\bar{x}}(C^n\phi\kappa_\alpha\delta_x\Big(\Big(C^n\phi)^{-1}\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S_\alpha^{n-1}\Big)\Big)_{ijk}\\
&+\delta_{\bar{y}}\Big(C^n\phi\kappa_\alpha\delta_y\Big((C^n\phi)^{-1}\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S_\alpha^{n-1}\Big)\Big)_{ijk}\Big\}\\
&+(\Delta t_c)^2\delta_{\bar{x}}\Big(C^n\phi\kappa_\alpha\delta_x\Big((C^n\phi)^{-1}\delta_{\bar{y}}\Big(C^n\phi\kappa_\alpha\delta_y\Big((C^n\phi)^{-1}\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S_\alpha^{n-1}\Big)\Big)\Big)\Big)_{ijk},\\
&\qquad\qquad X_{ijk}\in\Omega_h,\quad \alpha=1,2,\cdots,n_c, \qquad (4.25a)\\
&S_{\alpha,ijk}^n=h_{\alpha,ijk}^n,\quad X_{ijk}\in\partial\Omega_h,\quad \alpha=1,2,\cdots,n_c. \qquad (4.25b)
\end{aligned}
$$

Error equation is concluded from (1.6) ($t=t^n$) and (4.25),

$$
\begin{aligned}
&\phi_{ijk}C_{ijk}^n\frac{\xi_{\alpha,ijk}^n-\xi_{\alpha,ijk}^{n-1}}{\Delta t_c}-\sum_{r=x,y,z}\delta_{\bar{s}}(C^n\phi\kappa_\alpha\delta_r\xi_\alpha^n)_{ijk}\\
&=\Big\{\phi(C^n-c^n)\frac{\partial s_\alpha^n}{\partial t}\Big\}_{ijk}+\sum_{r=x,y,z}\delta_{\bar{r}}((c^n-C^n)\phi\kappa_\alpha\delta_r s_\alpha^n)_{ijk}+\sum_{r=x,y,z}\{\delta_{E\mathbf{U}^n,r}S_\alpha^n-\delta_{\mathbf{u}^n,r}s_\alpha^n\}_{ijk}\\
&\quad+Q_\alpha(c_{ijk}^n,s_{\alpha,ijk}^{n-1})-Q_\alpha(C_{ijk}^n,S_{\alpha,ijk}^{n-1})+\Big\{(S_\alpha-s_\alpha)q^n+\Big(S_\alpha^{n-1}\phi\frac{C^n-C^{n-1}}{\Delta t_c}-s_\alpha^n\phi\frac{\partial c^n}{\partial t}\Big)\Big\}_{ijk}\\
&\quad-(\Delta t_c)^2\Big\{\delta_{\bar{x}}(c^n\phi\kappa_\alpha\delta_x((c^n\phi)^{-1}\delta_{\bar{y}}(c^n\phi\kappa_\alpha\delta_y(d_ts_\alpha^{n-1}))))_{ijk}\\
&\quad-\delta_{\bar{x}}(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1}\delta_{\bar{y}}(C^n\phi\kappa_\alpha\delta_y(d_tS_\alpha^{n-1}))))_{ijk}+\cdots\Big\}\\
&\quad+(\Delta t_c)^3\{\delta_{\bar{x}}(c^n\phi\kappa_\alpha\delta_x((c^n\phi)^{-1}\delta_{\bar{y}}(c^n\phi\kappa_\alpha\delta_y((c^n\phi)^{-1}\delta_{\bar{z}}(c^n\phi\kappa_\alpha\delta_z(d_ts_\alpha^{n-1}))))))_{ijk}\\
&\quad-\delta_{\bar{x}}(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1}\delta_{\bar{y}}(C^n\phi\kappa_\alpha\delta_y((C^n\phi)^{-1}\delta_{\bar{z}}(C^n\phi\kappa_\alpha\delta_z(d_tS_\alpha^{n-1}))))))_{ijk}\}\\
&\quad-\Delta t_c\Big\{\Big[\delta_{\bar{x}}\Big(c^n\phi\kappa_\alpha\delta_x((c^n\phi)^{-1})+\delta_{\bar{y}}(c^n\phi\kappa_\alpha\delta_y((c^n\phi)^{-1})\Big]\sum_{r=x,y,z}\delta_{\mathbf{u}^n,r}s_\alpha^{n-1}\Big)\Big)_{ijk}\\
&\quad-\Big[\delta_{\bar{x}}\Big(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1})+\delta_{\bar{y}}\Big(C^n\phi\kappa_\alpha\delta_y((C^n\phi)^{-1})\Big]\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S_\alpha^{n-1}\Big)\Big)_{ijk}\Big\}\\
&\quad+(\Delta t_c)^2\Big\{\delta_{\bar{x}}\Big(c^n\phi\kappa_\alpha\delta_x\Big((c^n\phi)^{-1}\delta_{\bar{y}}\Big(c^n\phi\kappa_\alpha\delta_y\Big((c^n\phi)^{-1}\sum_{r=x,y,z}\delta_{\mathbf{u}^n,r}s_\alpha^{n-1}\Big)\Big)\Big)\Big)_{ijk}\\
&\quad-\delta_{\bar{x}}\Big(C^n\phi\kappa_\alpha\delta_x\Big((C^n\phi)^{-1}\delta_{\bar{y}}\Big(C^n\phi\kappa_\alpha\delta_y\Big((C^n\phi)^{-1}\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S_\alpha^{n-1})\Big)\Big)\Big)_{ijk}\Big\}\\
&\quad+\varepsilon_{\alpha,ijk},\quad X_{ijk}\in\Omega_h,\quad \alpha=1,2,\cdots,n_c, \qquad (4.26a)\\
&\xi_{\alpha,ijk}^n=0,\quad X_{ijk}\in\partial\Omega_h,\quad \alpha=1,2,\cdots,n_c, \qquad (4.26b)
\end{aligned}
$$

where

$$\left|\varepsilon_{\alpha,ijk}^{n+1}\right| \le K\left\{h_s^2+\Delta t_c\right\}, \quad \alpha=1,2,\cdots,n_c.$$

Noting that bound water exists everywhere, so we have that $c(X,t)\ge c_*>0$ for a positive constant c_*. The concentration of water $c(X,t)$ is estimated by (4.24). If h_c and Δt_c are sufficiently small, then

$$C(X,t)\ge \frac{c_*}{2}. \tag{4.27a}$$

$C(X,t)$ has the following regularity,

$$\sup_n\left|d_tC^{n-1}\right|_\infty \le K^*, \tag{4.27b}$$

where K^* is a positive constant.

Multiplying both sides of (4.26) by

$$\delta_t\xi_{\alpha,ijk}^{n-1}=d_t\xi_{\alpha,ijk}^{n-1}\Delta t_c=\xi_{\alpha,ijk}^{n}-\xi_{\alpha,ijk}^{n-1},$$

we get

$$\begin{aligned}
&\left\langle \phi C^n\frac{\xi_\alpha^n-\xi_\alpha^{n-1}}{\Delta t_c},d_t\xi_\alpha^{n-1}\right\rangle\Delta t_c+\sum_{r=x,y,z}\left\langle C^n\phi\kappa_\alpha\delta_r\xi_\alpha^n,\delta_r(\xi_\alpha^n-\xi_\alpha^{n-1})\right\rangle\\
=&\left\langle \phi(C^n-c^n)\frac{\partial s_\alpha^n}{\partial t},d_t\xi_\alpha^{n-1}\right\rangle\Delta t_c+\sum_{r=x,y,z}\left\langle \delta_{\bar r}((c^n-C^n)\phi\kappa_\alpha\delta_r s_\alpha^n),d_t\xi_\alpha^{n-1}\right\rangle\Delta t_c\\
&+\sum_{r=x,y,z}\left\langle \delta_{E\mathbf{U}^n,r}S_\alpha^n-\delta_{\mathbf{u}^n,r}s_\alpha^n,d_t\xi_\alpha^{n-1}\right\rangle\Delta t_c+\left\langle Q_\alpha(c^n,s_\alpha^{n-1})-Q_\alpha(C^n,S_\alpha^{n-1}),d_t\xi_\alpha^{n-1}\right\rangle\Delta t_c\\
&+\left\langle q^n(S_\alpha-s_\alpha),d_t\xi_\alpha^{n-1}\right\rangle\Delta t_c+\left\langle S_\alpha^{n-1}\phi\frac{C^n-C^{n-1}}{\Delta t_c}-s_\alpha^n\phi\frac{\partial c^n}{\partial t},d_t\xi_\alpha^{n-1}\right\rangle\Delta t_c\\
&-(\Delta t_c)^3\Big\{\Big\langle \delta_{\bar x}(c^n\phi\kappa_\alpha\delta_x((c^n\phi)^{-1}\delta_{\bar y}(c^n\phi\kappa_\alpha\delta_y(d_ts_\alpha^{n-1}))))\\
&-\delta_{\bar x}(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1}\delta_{\bar y}(C^n\phi\kappa_\alpha\delta_y(d_tS_\alpha^{n-1})))),d_t\xi_\alpha^{n-1}\Big\rangle+\cdots\Big\}\\
&+(\Delta t_c)^4\Big\langle \delta_{\bar x}(c^n\phi\kappa_\alpha\delta_x((c^n\phi)^{-1}\delta_{\bar y}(c^n\phi\kappa_\alpha\delta_y((c^n\phi)^{-1}\delta_{\bar z}(c^n\phi\kappa_\alpha\delta_z(d_ts_\alpha^{n-1}))))))\\
&-\delta_{\bar x}(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1}\delta_{\bar y}(C^n\phi\kappa_\alpha\delta_y((C^n\phi)^{-1}\delta_{\bar z}(C^n\phi\kappa_\alpha\delta_z(d_tS_\alpha^{n-1})))))),d_t\xi_\alpha^{n-1}\Big\rangle\\
&-(\Delta t_c)^2\Big\langle\Big[\delta_{\bar x}\Big(c^n\phi\kappa_\alpha\delta_x((c^n\phi)^{-1})+\delta_{\bar y}(c^n\phi\kappa_\alpha\delta_y((c^n\phi)^{-1})\Big]\sum_{r=x,y,z}\delta_{\mathbf{u}^n,r}s_\alpha^{n-1}\Big)\Big)\\
&-\Big[\delta_{\bar x}\Big(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1})+\delta_{\bar y}(C^n\phi\kappa_\alpha\delta_y((C^n\phi)^{-1})\Big]\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S_\alpha^{n-1}\Big)\Big),d_t\xi_\alpha^{n-1}\Big\rangle\\
&+(\Delta t_c)^3\Big\langle\delta_{\bar x}\Big(c^n\phi\kappa_\alpha\delta_x\Big((c^n\phi)^{-1}\delta_{\bar y}\Big(c^n\phi\kappa_\alpha\delta_y\Big((c^n\phi)^{-1}\sum_{r=x,y,z}\delta_{\mathbf{u}^n,r}s_\alpha^{n-1})\Big)\Big)\Big)
\end{aligned}$$

$$-\delta_{\bar{x}}\Big(C^n\phi\kappa_\alpha\delta_x\Big(\big(C^n\phi\big)^{-1}\delta_{\bar{y}}\Big(C^n\phi\kappa_\alpha\delta_y\Big(\big(C^n\phi\big)^{-1}\sum_{r=x,y,z}\delta_{E\mathbf{U}^n,r}S_\alpha^{n-1}\Big)\Big)\Big)\Big),d_t\xi_\alpha^{n-1}\Big\rangle$$
$$+\Big\langle\varepsilon_\alpha,d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c. \tag{4.28}$$

The left-hand side terms of (4.28) are estimated as follows

$$\Big\langle\phi C^n d_t\xi_\alpha^{n-1},d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c\geq\frac{1}{2}\phi_*c_*\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2\Delta t_c, \tag{4.29a}$$

$$\sum_{r=x,y,z}\Big\langle C^n\phi\kappa_\alpha\delta_r\xi_\alpha^n,\delta_r(\xi_\alpha^n-\xi_\alpha^{n-1})\Big\rangle$$
$$\geq\frac{1}{2}\sum_{r=x,y,z}\Big\{\Big\langle C^n\phi\kappa_\alpha\delta_r\xi_\alpha^n,\delta_r\xi_\alpha^n\Big\rangle-\Big\langle C^n\phi\kappa_\alpha\delta_r\xi_\alpha^{n-1},\delta_r\xi_\alpha^{n-1}\Big\rangle\Big\}. \tag{4.29b}$$

The right-hand side terms of (4.28) are estimated,

$$\Big\langle\phi(C^n-c^n)\frac{\partial s_\alpha^n}{\partial t},d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2\Delta t_c+K\big\{h_c^2+(\Delta t_c)^2\big\}, \tag{4.30a}$$

$$\sum_{r=x,y,z}\Big\langle\delta_{\bar{r}}((c^n-C^n)\phi\kappa_\alpha\delta_r s_\alpha^n),d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2+K\big\{h_c^2+(\Delta t_c)^2\big\}, \tag{4.30b}$$

$$\sum_{r=x,y,z}\Big\langle\delta_{E\mathbf{U}^n,r}S_\alpha^n-\delta_{\mathbf{u}^n,r}s_\alpha^n,d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c$$
$$\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2\Delta t_c+K\big\{\big|\big|\nabla_h\xi_\alpha^n\big|\big|^2+h_c^2+(\Delta t_c)^2\big\}\Delta t_c, \tag{4.30c}$$

$$\Big\langle Q_\alpha(c^n,s_\alpha^{n-1})-Q_\alpha(C^n,S_\alpha^{n-1}),d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c$$
$$\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2\Delta t_c+K\big\{\big|\big|\xi_\alpha^n\big|\big|^2+h_c^2+(\Delta t_c)^2\big\}\Delta t_c, \tag{4.30d}$$

$$\Big\langle q^n(S_\alpha-s_\alpha),d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2\Delta t_c+K\big\{\big|\big|\xi_\alpha^n\big|\big|^2+(\Delta t_c)^2\big\}\Delta t_c, \tag{4.30e}$$

$$\Big\langle S_\alpha^{n-1}\phi\frac{C^n-C^{n-1}}{\Delta t_c}-s_\alpha^n\phi\frac{\partial c^n}{\partial t},d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c$$
$$\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2\Delta t_c+K\big\{\big|\big|\xi_\alpha^n\big|\big|^2+h_c^2+(\Delta t_c)^2\big\}, \tag{4.30f}$$

$$-(\Delta t_c)^3\Big\{\Big\langle\delta_{\bar{x}}(c^n\phi\kappa_\alpha\delta_x((c^n\phi)^{-1}\delta_{\bar{y}}(c^n\phi\kappa_\alpha\delta_y(d_t s_\alpha^{n-1}))))$$
$$-\delta_{\bar{x}}(C^n\phi\kappa_\alpha\delta_x((C^n\phi)^{-1}\delta_{\bar{y}}(C^n\phi\kappa_\alpha\delta_y(d_t S_\alpha^{n-1})))),d_t\xi_\alpha^{n-1}\Big\rangle+\cdots\Big\}+\cdots+\Big\langle\varepsilon_\alpha,d_t\xi_\alpha^{n-1}\Big\rangle\Delta t_c$$
$$\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2+K\big\{\big|\big|\nabla_h\xi_\alpha^n\big|\big|^2+h_c^2+h_s^4+(\Delta t_c)^2\big\}\Delta t_c. \tag{4.30g}$$

Substituting (4.29) and (4.30) into (4.28), we have

$$\frac{1}{2}\phi_*c_*\Big|\Big|d_t\xi_\alpha^{n-1}\Big|\Big|^2\Delta t_c+\frac{1}{2}\sum_{r=x,y,z}\Big\{\Big\langle C^n\phi\kappa_\alpha\delta_r\xi_\alpha^n,\delta_r\xi_\alpha^n\Big\rangle-\Big\langle C^n\phi\kappa_\alpha\delta_r\xi_\alpha^{n-1},\delta_r\xi_\alpha^{n-1}\Big\rangle\Big\}$$
$$\leq\varepsilon\big|\big|d_t\xi_\alpha^{n-1}\big|\big|^2+K\big\{\big|\big|\nabla_h\xi_\alpha^n\big|\big|^2+\big|\big|\xi_\alpha^n\big|\big|^2+h_c^2+h_s^4+(\Delta t_c)^2\big\}\Delta t_c. \tag{4.31}$$

Summing on n $(0<n\le L)$, and noting that $\xi_\alpha^0=0$, we have

$$\begin{aligned}&\sum_{n=0}^{L}||d_t\xi_\alpha^{n-1}||^2\Delta t_c+\sum_{r=x,y,z}\Big\{\Big\langle C^L\phi\kappa_\alpha\delta_r\xi_\alpha^L,\delta_r\xi_\alpha^L\Big\rangle-\Big\langle C^0\phi\kappa_\alpha\delta_r\xi_\alpha^0,\delta_r\xi_\alpha^0\Big\rangle\Big\}\\ \le&\sum_{n=0}^{L}\sum_{r=x,y,z}\Big\langle[C^n-C^{n-1}]\phi\kappa_\alpha\delta_r\xi_\alpha^n,\delta_r\xi_\alpha^n\Big\rangle\\ &+K\sum_{n=0}^{L}\Big\{||\nabla_h\xi_\alpha^n||^2+||\xi_\alpha^n||^2+h_c^2+h_s^4+(\Delta t_c)^2\Big\}\Delta t_c. \end{aligned}\tag{4.32}$$

The first term on the right-hand side of (4.32) is estimated by

$$\sum_{n=0}^{L}\sum_{r=x,y,z}\Big\langle[C^n-C^{n-1}]\phi\kappa_\alpha\delta_r\xi_\alpha^n,\delta_r\xi_\alpha^n\Big\rangle\le K\sum_{n=0}^{L}||\nabla_h\xi_\alpha^n||^2\Delta t_c.\tag{4.33}$$

Then,

$$\sum_{n=1}^{L}||d_t\xi_\alpha^{n-1}||^2\Delta t_c+||\nabla_h\xi_\alpha^L||^2\le K\sum_{n=0}^{L}\Big\{||\nabla_h\xi_\alpha^n||^2+||\xi_\alpha^n||^2+h_c^2+h_s^4+(\Delta t_c)^2\Big\}\Delta t_c.\tag{4.34}$$

The fact that $\xi_\alpha^0=0$ indicates

$$||\xi_\alpha^L||^2\le\varepsilon\sum_{n=1}^{L}||d_t\xi_\alpha^{n-1}||^2\Delta t_c+K\sum_{n=0}^{L}||\xi_\alpha^n||^2\Delta t_c.$$

Thus,

$$\sum_{n=1}^{L}||d_t\xi_\alpha^{n-1}||^2\Delta t_c+||\xi_\alpha^L||_1^2\le K\sum_{n=0}^{L}\Big\{||\xi_\alpha^n||^2+h_c^2+h_s^4+(\Delta t_c)^2\Big\}\Delta t_c,\tag{4.35}$$

where

$$||\xi_\alpha||_1^2=||\xi_\alpha||^2+||\nabla_h\xi_\alpha||^2.$$

Applying the Gronwall Lemma, we have

$$\sum_{n=1}^{L}||d_t\xi_\alpha^{n-1}||^2\Delta t_c+||\xi_\alpha^L||_1^2\le K\Big\{h_c^2+h_s^4+(\Delta t_c)^2\Big\},\quad \alpha=1,2,\cdots,n_c.\tag{4.36}$$

The following theorem is concluded by using (4.23), (4.24), (4.36) and Lemma 4.1.

Theorem 4.1. *Suppose that exact solutions of* (1.1)-(1.5) *are regular (R), and the coefficients are positive definite (C). Numerical solutions are obtained by using the composite scheme of* (3.4), (3.6) *and* (3.13)-(3.15). *Then,*

$$\begin{aligned}&||p-P||_{\bar L^\infty(J;\bar m)}+||\mathbf{u}-\mathbf{U}||_{\bar L^\infty(J;V)}+||c-C||_{\bar L^\infty(J;\bar m)}+||\bar{\mathbf{z}}-\bar{\mathbf{Z}}||_{\bar L^2(J;V)}\\ &+\sum_{\alpha=1}^{n_c}\Big\{||d_t(s_\alpha-S_\alpha)||_{\bar L^2(J;l^2)}+||s_\alpha-S_\alpha||_{\bar L^\infty(J;h^1)}\Big\}\\ \le&M^*\Big\{h_p^2+h_c+h_s^2+\Delta t_c+(\Delta t_{p,1})^{3/2}+(\Delta t_p)^2\Big\},\end{aligned}\tag{4.37}$$

where

$$||g||_{\bar{L}^\infty(J;\mathbf{X})}=\sup_{n\Delta t\le T}||g^n||_{\mathbf{X}},\quad ||g||_{\bar{L}^2(J;\mathbf{X})}=\sup_{L\Delta t\le T}\left\{\sum_{n=0}^{L}||g^n||^2_{\mathbf{X}}\Delta t\right\}^{1/2},$$

and the constant M^* depends on p, c, s_α $(\alpha=1,2,\cdots,n_c)$ and their derivatives.

5 Numerical experiments

In this section, a nonlinear system is considered by using the presented scheme. The mathematical model is defined as follows

$$\begin{cases} -\nabla\cdot(D_1(c,t)\nabla p)=f_1, & (x,y,z)\in\Omega, \quad t\in(0,T],\\ \mathbf{u}=-D_1(c,t)\nabla p, & (x,y,z)\in\Omega, \quad t\in(0,T],\\ \dfrac{\partial c}{\partial t}-\nabla\cdot(D_2(\mathbf{u})\nabla c)+\mathbf{u}\cdot\nabla c=f_2, & (x,y,z)\in\Omega, \quad t\in(0,T],\\ \dfrac{\partial s}{\partial t}-\nabla\cdot(D_3(c)\nabla s)+\mathbf{u}\cdot\nabla s=f_3, & (x,y,z)\in\Omega, \quad t\in(0,T],\\ p(x,y,z,0)=p_0(x,y,z), & (x,y,z)\in\Omega,\\ c(x,y,z,0)=c_0(x,y,z), & (x,y,z)\in\Omega,\\ s(x,y,z,0)=s_0(x,y,z), & (x,y,z)\in\Omega,\\ \nabla c\cdot\gamma|_{\partial\Omega}=0, & t\in(0,T],\\ \nabla s\cdot\gamma|_{\partial\Omega}=0, & t\in(0,T]. \end{cases} \tag{5.1}$$

$\Omega=[0,1]\times[0,1]\times[0,1]$. Exact solutions are defined by

$$\begin{aligned} &p(x,y,z,t)=\exp(-\pi^2 t)\big(x(x-1)y(y-1)z(z-1)\big)^2,\\ &c(x,y,z,t)=\exp(-2t)\cos(2\pi x)\cos(2\pi y)\cos(2\pi z),\\ &s(x,y,z,t)=\exp(-t^2)\cos(\pi x)\cos(\pi y)\cos(\pi z), \end{aligned}$$

with initial values

$$\begin{aligned} &p_0(x,y,z)=\big(x(x-1)y(y-1)z(z-1)\big)^2,\\ &c_0(x,y,z)=\cos(2\pi x)\cos(2\pi y)\cos(2\pi z),\\ &s_0(x,y,z)=\cos(\pi x)\cos(\pi y)\cos(\pi z). \end{aligned}$$

p, $\mathbf{u}$ c and s denote the pressure, Darcy velocity, concentration and saturation of a component. The diffusions are defined by

$$D_1(c,t)=15+10c,$$

$$D_2(\mathbf{u})=0.1+10^{-3}\mathbf{u}=\begin{pmatrix} 0.1+10^{-3}D_1(c)\dfrac{\partial p}{\partial x} & 0 & 0 \\ 0 & 0.1+10^{-3}D_1(c)\dfrac{\partial p}{\partial y} & 0 \\ 0 & 0 & 0.1+10^{-3}D_1(c)\dfrac{\partial p}{\partial z} \end{pmatrix},$$

$$D_3(c,t)=0.1+10^{-3}c.$$

f_1, f_2 and f_3 are the right-hand functions. An upwind block-centered scheme is used for solving (5.1). The experiments are carried out on the MATLAB 2018a (MathWorks, Natick, MA). The partition is uniform with space step $h=1/N$ and time size $\Delta t=h^2$. Take $T=0.1$. N is a positive integer. P, $\mathbf{U}$, C and S denote numerical approximations of p, $\mathbf{u}$, c and s. Error estimates are illustrated in Tables 1-3. Let

$$M_p=\max_{i,j,k,n}|p^n_{ijk}-P^n_{ijk}|,\quad E_p=\Big(\sum_{i,j,k}|p^n_{ijk}-P^n_{ijk}|^2h^3\Big)^{1/2},\quad RE_p=E_p\Big(\sum_{i,j,k}|P^n_{ijk}|^2h^3\Big)^{-1/2},$$

denote the errors of the pressure p in the maximum norm, l^2-norm and their relative errors, respectively. Define M_c, M_s, E_c, E_s, RE_c and RE_s similarly. Error of Darcy velocity in l^2-norm is defined by

$$\begin{aligned}E^2_{\mathbf{u}}=&\sum_{i,j,k}(u_{1,i-1/2,jk}-U_{1,i-1/2,jk})^2h^3+\sum_{i,j,k}(u_{2,i,j-1/2,k}-U_{2,i,j-1/2,k})^2h^3\\&+\sum_{i,j,k}(u_{3,ij,k-1/2}-U_{3,ij,k-1/2})^2h^3.\end{aligned}$$

$RE_{\mathbf{u}}=E_{\mathbf{u}}/|||\mathbf{U}|||$ denotes relative error, where

$$|||\mathbf{U}|||^2=\sum_{i,j,k}U^2_{1,i-1/2,jk}h^3+\sum_{i,j,k}U^2_{2,i,j-1/2,k}h^3+\sum_{i,j,k}U^2_{3,ij,k-1/2}h^3.$$

From the tables, we find that the presented method is valid for solving (5.1). Numerical results are consistent with theoretical results. Thus, some complicated problems are possibly solved by this method.

Table 1: Error estimates.

N	10	20	40	50	80
M_p	6.4364e−6	1.6002e−6	4.0191e−7	2.5712e−7	1.0031e−7
E_p	2.8766e−6	7.1626e−7	1.7884e−7	1.1442e−7	4.4636e−8
M_c	1.8102e−2	5.1966e−3	1.3446e−3	8.6411e−4	3.3906e−4
E_c	7.3369e−3	1.8829e−3	4.7392e−4	3.0355e−4	1.1868e−4
M_s	1.2425e−3	3.2695e−4	8.2799e−5	5.3073e−5	2.066e−5
E_s	4.2742e−4	1.0781e−4	2.7014e−5	1.7294e−5	6.7576e−6

Table 2: Relative error estimates.

N	10	20	40	50	80
RE_p	$4.4934e-2$	$1.1559e-2$	$2.9103e-3$	$1.8638e-3$	$7.2785e-4$
RE_c	$2.4720e-2$	$6.4629e-3$	$1.6345e-3$	$1.0475e-3$	$4.0983e-4$
RE_s	$1.2196e-3$	$3.0792e-4$	$7.7171e-5$	$4.9404e-5$	$1.9305e-5$

Table 3: Error estimates of Darcy velocity.

N	10	20	40	50	80
$E_{\mathbf{u}}$	$3.4800e-5$	$1.8619e-5$	$9.5391e-6$	$7.6632e-6$	$4.8191e-6$
$RE_{\mathbf{u}}$	$7.9746e-3$	$2.0284-3$	$5.1297e-4$	$3.2917e-4$	$1.2916e-4$

6 Conclusions and discussions

An upwind block-centered fractional step difference method is proposed and theoretical analysis is presented. Three-dimensional seepage displacement of chemical oil recovery in porous media is discussed in this paper. Several interesting conclusions are stated as follows.

(I) The scheme has the conservation of mass, which is an important nature in numerical simulation of seepage mechanics especially for chemical oil recovery.

(II) The numerical method combines block-centered difference, upwind approximation and fractional step difference, so it has high accuracy and strong stability. Furthermore, it is easily to be used for solving large-scale actual engineering problems on three-dimensional complicated region.

(III) The boundary conditions are treated simply for the presented scheme and the applications are carried out easily.

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