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An Upwind Mixed Volume Element-Fractional Step Method on a Changing Mesh for Compressible Contamination Treatment from Nuclear Waste

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Abstract. In this paper the authors discuss the numerical simulation problem of three-dimensional compressible contamination treatment from nuclear waste. The mathematical model is defined by an initial-boundary nonlinear convection-diffusion system of four partial differential equations: a parabolic equation for the pressure, two convection-diffusion equations for the concentrations of brine and radionuclide and a heat conduction equation for the temperature. The pressure appears within the concentration equations and heat conduction equation, and the Darcy velocity controls the concentrations and the temperature. The pressure is solved by the conservative mixed volume element method, and the order of the accuracy is improved by the Darcy velocity. The concentration of brine and temperature are computed by the upwind mixed volume element method on a changing mesh, where the diffusion is discretized by a mixed volume element and the convection is treated by an upwind scheme. The composite method can solve the convection-dominated diffusion problems well because it eliminates numerical dispersion and nonphysical oscillation and has high order computational accuracy. The mixed volume element has the local conservation of mass and energy, and it can obtain the brine and temperature and their adjoint vector functions simultaneously. The conservation nature plays an important role in numerical simulation of underground fluid. The concentrations of radionuclide factors are solved by the method of upwind fractional step difference and the computational work is decreased by decomposing a three-dimensional problem into three successive one-dimensional problems and using the method of speedup. By the theory and technique of a priori estimates of differential equations, we derive an optimal order result in L^2 norm. Numerical examples are given to show the effectiveness and practicability and the composite method is testified as a powerful tool to solve the well-known actual problem.

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1 Introduction

An upwind mixed volume element-fractional step difference method on a changing mesh is proposed and its numerical analysis is shown in this paper for compressible nuclear waste contamination disposal in porous media. High-level nuclear waste in underground repositories is diffused and gives destructive disaster once natural disaster, such as earthquake or rock fracture, takes place. So it is important to understand how the pollution spreads and to obtain the safeguard measures. Numerical simulation of this problem plays an important role in modern energy mathematics, and the research on computational method of nuclear waste in porous media can give valuable suggestions for disposing and analyzing the contamination. The compressible three-dimensional mathematical model is formulated by an initial-boundary system of coupled convection-diffusion partial differential equations to describe the transport in underground environment. The physical features are stated by the movement of flow, the heat conduction migration, the miscible displacement of main contamination (brine) and the miscible displacement of trace contamination factors (radionuclide). The mathematical description is stated below following the work on slight-compressibility by Douglas [1–3].

Fluid:

$$\phi_1\frac{\partial p}{\partial t}+\nabla\cdot\mathbf{u}=-q+R_s', \qquad X=(x,y,z)^T\in\Omega, \quad t\in J=(0,\bar{T}], \tag{1.1a}$$

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

where $p(X,t)$ and $\mathbf{u}(X,t)$ are the fluid pressure and Darcy velocity, respectively. $\phi_1=\phi c_w$, and $q=q(X,t)$ is the production. $R_s'=R_s'(\hat{c})=[c_s\phi K_s f_s/(1+c_s)](1-\hat{c})$ is a salt dissolution term of main contamination, $\kappa(X)$ is the permeability of the rock, and $\mu(\hat{c})$ is the viscosity dependent on the concentration of main contamination $\hat{c}$.

Heat:

$$d_1(p)\frac{\partial p}{\partial t}+d_2\frac{\partial T}{\partial t}+c_p\mathbf{u}\cdot\nabla T-\nabla\cdot(E_H\nabla T)=Q(\mathbf{u},p,T,\hat{c}), \quad X\in\Omega, \quad t\in J, \tag{1.2}$$

where T is the temperature. I denotes an identity matrix, $d_1(p)=\phi c_w[v_0+(p/\rho)]$, $d_2=\phi c_p+(1-\phi)\rho_R\rho_{pR}$, $E_H=Dc_{pw}+K_m'I$, $K_m'=\kappa_m/\rho_o$. $D=(D_{ij})=(\alpha_T|\mathbf{u}|\delta_{ij}+(\alpha_L-\alpha_T)u_iu_j/|\mathbf{u}|)$, $Q(\mathbf{u},p,T,\hat{c})=-\{[\nabla v_0-c_p\nabla T_0]\cdot\mathbf{u}+[v_0+c_p(T-T_0)+(p/\rho)][-q+R_s']\}-q_L-qH-q_H$. Take $E_H=K_m'I$ in general.

The concentration of brine (main contamination):

$$\phi\frac{\partial\hat{c}}{\partial t}+\mathbf{u}\cdot\nabla\hat{c}-\nabla\cdot(E_c\nabla\hat{c})=f(\hat{c}), \quad X\in\Omega, \quad t\in J, \tag{1.3}$$

where ϕ is the porosity, $E_c=D+D_mI$, $E_c=D+D_mI$, $f(\hat{c})=-\hat{c}\{[c_s\phi K_sf_s/(1+c_s)](1-\hat{c})\}-q_c-R_s$. Take $E_c=D_mI$.

The concentrations of radionuclide (trace contamination factors):

$$\begin{aligned}&\phi K_l\frac{\partial c_l}{\partial t}+\mathbf{u}\cdot\nabla c_l-\nabla\cdot(E_c\nabla c_l)+d_3(c_l)\frac{\partial p}{\partial t}\\&=f_l(\hat{c},c_1,c_2,\cdots,c_N),\quad X\in\Omega,\quad t\in J,\quad l=1,2,\cdots,N,\end{aligned}\tag{1.4}$$

where c_l denotes the concentration of l-th trace contamination $(l=1,2,\cdots,N)$, $d_3(c_l)=\phi c_w c_l(K_l-1)$, and $f_l(\hat{c},c_1,c_2,\cdots,c_N)=c_l\{q-[c_s\phi K_sf_s/(1+c_s)](1-\hat{c})\}-qc_l-q_{c_l}+q_{ol}+\sum_{j=1}^{N}k_j\lambda_jK_j\phi c_j-\lambda_lK_l\phi c_l$.

We assume that no flow of fluid occurs across the boundary (Impermeable boundary conditions):

$$\mathbf{u}\cdot\nu=0,\qquad (X,t)\in\partial\Omega\times J,\tag{1.5a}$$

$$(E_c\nabla\hat{c}-\hat{c}\mathbf{u})\cdot\nu=0,\qquad (X,t)\in\partial\Omega\times J,\tag{1.5b}$$

$$(E_c\nabla c_l-c_l\mathbf{u})\cdot\nu=0,\qquad (X,t)\in\partial\Omega\times J,\quad l=1,2,\cdots,N.\tag{1.5c}$$

Ω is a bounded domain of R^3, and ν is the outer normal vector to the boundary surface $\partial\Omega$. No heat transports across the boundary of (1.2)

$$(E_H\nabla T-c_p\mathbf{u})\cdot\nu=0,\quad (X,t)\in\partial\Omega\times J.\tag{1.5d}$$

Furthermore, initial conditions are given as follows

$$p(X,0)=p_0(X),\quad \hat{c}(X,0)=\hat{c}_0(X),\quad c_l(X,0)=c_{l0}(X),\quad l=1,2,\cdots,N,\tag{1.6a}$$

$$T(X,0)=T_0(X),\quad X\in\Omega.\tag{1.6b}$$

Douglas, Ewing, Russell, Wheeler and Yuan gave a series of research on the incompressible two-phase displacement problem [3–8]. For modern numerical simulation of energy and environmental sciences especially of seepage transportation, the compressibility must be considered to avoid numerical distortion [9, 10]. Douglas and Yuan et al. proposed several numerical methods for solving two-phase compressible displacement problem [3, 8, 11, 12] such as the method of characteristic finite element [8, 13, 14], the characteristic finite difference [15,16], fractional step differences [8,17]. The finite volume element method [18, 19] has some advantages, such as the simplicity of the difference method, the high-order accuracy of the finite element method and the local conservation of mass, so it is an effective method to solve partial differential equations. The mixed finite element method was argured in [20–22] for solving the pressure and Darcy velocity simultaneously and the accuracy was improved by one order. A mixed volume element combining the above two methods was discussed in [3, 23, 24], and numerical experiments were presented in [25, 26] to demonstrate the efficiency. Theoretical analysis was given for an elliptic problem in [27–29], along with a general discussion of the form of the mixed volume element method. Rui and Pan adopted this method to argue numerical computation for Darcy-Forchheimer flow problems in [30, 31]. On numerical simulation of nuclear waste disposal problem, Yuan and Ewing studied the methods of finite element and finite difference carefully and discussed the actual applications [2,9,12]. Adaptive finite element method, whereby the mesh changes dynamically during the simulation, has become an important tool to solve partial differential equations efficiently and accurately. Numerical solutions at some sharp bumps on special regions can be approximated excellently. In [32], Dawson and Kirby developed a backward-Euler mixed finite element method to solve the heat equation on dynamically changing meshes, and demonstrated that numerical solutions approached exact solutions in an optimal rate under a special changing mesh. On the basis of the previous studies, an upwind mixed volume element-fractional step difference method on a changing mesh is proposed for three-dimensional nuclear waste contamination problem in this paper. The pressure and Darcy velocity are computed simultaneously by the conservative mixed volume element method, and the accuracy is improved by one order for the Darcy velocity. The concentration of brine and the temperature are computed by the upwind mixed volume element scheme on a dynamically changing mesh, where the upwind scheme and mixed volume element are used to approximate convection and diffusion, respectively. The composite scheme can avoid numerical dispersion and decrease the time truncation error, so it works well in solving convection-dominated diffusion problems. The brine concentration and temperature and their adjoint vector functions are computed simultaneously. Since piece-wise-defined constant functions are taken as test functions, it has the nature of mass and energy conservation, an important law in numerical simulation of seepage mechanics. By the theory and special technique of a priori estimates of differential equations, we obtain optimal order error estimates. The concentrations of trace contamination factors, whose computational work is the largest, are treated by upwind fractional step differences. The computation on the whole domain is divided into three one-dimensional problems, where the algorithm of speedup is used [17]. In this paper numerical experiments are given for a simplified model problem of convection-diffusion equation, then numerical data show that this method is effective and support theoretical result. Moreover, this method gives an efficient tool for solving the challenging benchmark problem [1–3, 8, 17, 33, 34].

The common notation and norms of Sobolev space are adopted in this paper. The regularity assumptions of (1.1)-(1.6) are defined by

$$\text{(R)}\qquad \begin{cases} p\in L^\infty(H^1), \\ \mathbf{u}\in L^\infty(H^1(\text{div}))\bigcap L^\infty(W^1_\infty)\bigcap W^1_\infty(L^\infty)\bigcap H^2(L^2), \\ \hat{c}, c_l\,(l=1,2,\cdots,N),\ \ T\in L^\infty(H^2)\bigcap H^1(H^1)\bigcap L^\infty(W^1_\infty)\bigcap H^2(L^2). \end{cases}$$

We suppose that the coefficients of (1.1)-(1.6) satisfy the following positive definite conditions

$$\text{(C)}\qquad \begin{cases} 0<a_*\le\dfrac{\kappa(X)}{\mu(c)}\le a^*, \quad 0<\phi_*\le\phi,\phi_1\le\phi^*, \quad 0<d_*\le d_1,d_2,d_3\le d^*, \\ 0<K_*\le K_l\le K^*, \quad l=1,2,\cdots,N, \quad 0<E_*\le E_c\le E^*, \quad 0<\bar{E}_*\le E_H\le\bar{E}^*, \end{cases}$$

where a_*, a^*, ϕ_*, ϕ^*, d_*, d^*, K_*, K^*, E_*, E^*, $\bar{E}_*$ and $\bar{E}^*$ are positive constants. The coefficients are supposed to be bounded locally and be Lipschitz continuous.

In the following discussion 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 Notations and preparations

Three different partitions are constructed to define the method of upwind mixed volume element-fractional step differences on a changing mesh. The large-step partition is nonuniform for the pressure and Darcy velocity. The mid-step nonuniform partition dependent on t is defined to obtain the concentration of main contamination factor and the temperature, that is, the partitions maybe are different at different time levels. The small-step uniform partition is defined for the concentrations of trace contamination factors. The large-step and mid-step partitions are considered.

For simplicity, to discuss three-dimensional problems, take $\Omega=\{[0,1]\}^3$, and let $\partial\Omega$ denote the boundary. Define

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

Ω is partitioned by $\delta_x\times\delta_y\times\delta_z$. For $i=1,2,\cdots,N_x$, $j=1,2,\cdots,N_y$, and $k=1,2,\cdots,N_z$, let $\Omega_{ijk}=\{(x,y,z)|x_{i-1/2}<x<x_{i+1/2},y_{j-1/2}<y<y_{j+1/2},z_{k-1/2}<z<z_{k+1/2}\}$, $x_i=(x_{i-1/2}+x_{i+1/2})/2$, $y_j=(y_{j-1/2}+y_{j+1/2})/2$, $z_k=(z_{k-1/2}+z_{k+1/2})/2$. $h_{x_i}=x_{i+1/2}-x_{i-1/2}$, $h_{y_j}=y_{j+1/2}-y_{j-1/2}$, $h_{z_k}=z_{k+1/2}-z_{k-1/2}$. $h_{x,i+1/2}=(h_{x_i}+h_{x_{i+1}})/2=(x_{i+1/2}-x_{i-1/2})/2$, $h_{y,j+1/2}=(h_{y_j}+h_{y_{j+1}})/2=(y_{j+1/2}-y_{j-1/2})/2$, $h_{z,k+1/2}=(h_{z_k}+h_{z_{k+1}})/2=(z_{k+1/2}-z_{k-1/2})/2$. $h_x=\max_{1\le i\le N_x}\{h_{x_i}\}$, $h_y=\max_{1\le j\le N_y}\{h_{y_j}\}$, $h_z=\max_{1\le k\le N_z}\{h_{z_k}\}$, $h_p=(h_x^2+h_y^2+h_z^2)^{1/2}$. The partition is regular if there exist two positive constants α_1 and α_2 such that

$$\begin{aligned} &\min_{1\le i\le N_x}\{h_{x_i}\}\ge\alpha_1 h_x, \quad \min_{1\le j\le N_y}\{h_{y_j}\}\ge\alpha_1 h_y,\\ &\min_{1\le k\le N_z}\{h_{z_k}\}\ge\alpha_1 h_z, \quad \min\{h_x,h_y,h_z\}\ge\alpha_2\max\{h_x,h_y,h_z\}. \end{aligned}$$

Here α_1 and α_2 depend on the partition of Ω. A simple illustration of $N_x=4$, $N_y=3$ and $N_z=3$ is shown in Fig. 1. Define an experimental space by $M_l^d(\delta_x)=$

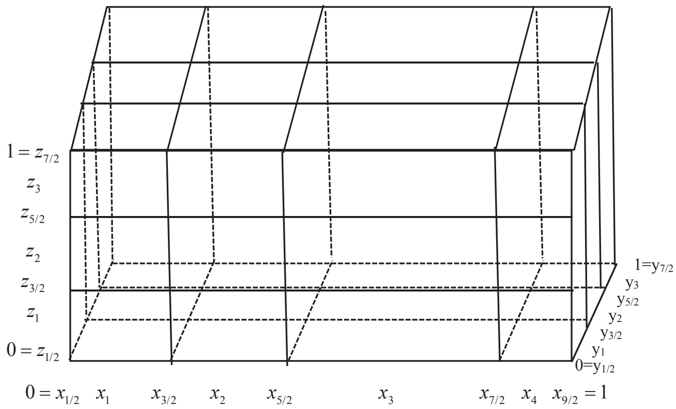

Figure 1: Nonuniform partition.

$\{f\in C^l[0,1]: f|_{\Omega_i}\in p_d(\Omega_i),\ i=1,2,\cdots,N_x\}$, where $\Omega_i=[x_{i-1/2},x_{i+1/2}]$ and $p_d(\Omega_i)$ denotes a space consisting of all the polynomial functions of degree at most d constricted on Ω_i. $f(x)$ is possibly discontinuous on $[0,1]$ if $l=-1$. $M_l^d(\delta_y)$ and $M_l^d(\delta_z)$ are defined similarly. Let $S_h=M_{-1}^0(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_{-1}^0(\delta_z)$, $V_h=\{\mathbf{w}|\mathbf{w}=(w^x,w^y,w^z),\ w^x\in M_0^1(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_{-1}^0(\delta_z),\ w^y\in M_{-1}^0(\delta_x)\bigotimes M_0^1(\delta_y)\bigotimes M_{-1}^0(\delta_z),\ w^z\in M_{-1}^0(\delta_x)\bigotimes M_{-1}^0(\delta_y)\bigotimes M_0^1(\delta_z)\ ,\ \mathbf{w}\cdot\mathbf{fl}|_{\partial\Omega}=0\}$. For a grid function $v(x,y,z)$, let v_{ijk}, $v_{i+1/2,jk}$, $v_{i,j+1/2,k}$ and $v_{ij,k+1/2}$ denote the values of $v(x_i,y_j,z_k)$, $v(x_{i+1/2},y_j,z_k)$, $v(x_i,y_{j+1/2},z_k)$ and $v(x_i,y_j,\ z_{k+1/2})$, respectively.

Inner products and norms are introduced,

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

Then a vector function $\mathbf{w}=(w^x,w^y,w^z)^T$ is measured by

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

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

$$||v||_m=||v||. \tag{2.1}$$

Introduce the difference operators and other notations as follows,

$$[d_xv]_{i+1/2,jk}=\frac{v_{i+1,jk}-v_{ijk}}{h_{x,i+1/2}},\qquad [d_yv]_{i,j+1/2,k}=\frac{v_{i,j+1,k}-v_{ijk}}{h_{y,j+1/2}},$$
$$[d_zv]_{ij,k+1/2}=\frac{v_{ij,k+1}-v_{ijk}}{h_{z,k+1/2}},\qquad [D_xw]_{ijk}=\frac{w_{i+1/2,jk}-w_{i-1/2,jk}}{h_{x_i}},$$
$$[D_yw]_{ijk}=\frac{w_{i,j+1/2,k}-w_{i,j-1/2,k}}{h_{y_j}},\qquad [D_zw]_{ijk}=\frac{w_{ij,k+1/2}-w_{ij,k-1/2}}{h_{z_k}},$$
$$\hat{w}^x_{ijk}=\frac{w^x_{i+1/2,jk}+w^x_{i-1/2,jk}}{2},\qquad \hat{w}^y_{ijk}=\frac{w^y_{i,j+1/2,k}+w^y_{i,j-1/2,k}}{2},$$
$$\hat{w}^z_{ijk}=\frac{w^z_{ij,k+1/2}+w^z_{ij,k-1/2}}{2},\qquad \bar{w}^x_{ijk}=\frac{h_{x,i+1}}{2h_{x,i+1/2}}w_{ijk}+\frac{h_{x,i}}{2h_{x,i+1/2}}w_{i+1,jk},$$
$$\bar{w}^y_{ijk}=\frac{h_{y,j+1}}{2h_{y,j+1/2}}w_{ijk}+\frac{h_{y,j}}{2h_{y,j+1/2}}w_{i,j+1,k},\qquad \bar{w}^z_{ijk}=\frac{h_{z,k+1}}{2h_{z,k+1/2}}w_{ijk}+\frac{h_{z,k}}{2h_{z,k+1/2}}w_{ij,k+1},$$

and $\hat{\mathbf{w}}_{ijk}=(\hat{w}^x_{ijk},\hat{w}^y_{ijk},\hat{w}^z_{ijk})^T$, $\bar{\mathbf{w}}_{ijk}=(\bar{w}^x_{ijk},\bar{w}^y_{ijk},\bar{w}^z_{ijk})^T$. $d_s(s=x,y,z)$ and $D_s(s=x,y,z)$ are difference quotient operators independent of the coefficient D in (1.3). Let L denote a positive integer, $\Delta t=T/L$, $t^n=n\Delta t$, $v^n=v(t^n)$ and $d_tv^n=(v^n-v^{n-1})/\Delta t$.

On the basis of the above notation, several preliminary statements are given.

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

$$\big(v,D_xw^x\big)_m=-\big(d_xv,w^x\big)_x,\quad \big(v,D_yw^y\big)_m=-\big(d_yv,w^y\big)_y,\quad \big(v,D_zw^z\big)_m=-\big(d_zv,w^z\big)_z. \tag{2.2}$$

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

$$||\hat{\mathbf{w}}||_m\leq|||\mathbf{w}|||. \tag{2.3}$$

Proof. It is required to prove $||\hat{w}^x||_m\leq||w^x||_x$, $||\hat{w}^y||_m\leq||w^y||_y$ and $||\hat{w}^z||_m\leq||w^z||_z$. From the fact that

$$\begin{aligned}
&\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x_i}h_{y_j}h_{z_k}(\hat{w}^x_{ijk})^2\\
\le&\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{y_j}h_{z_k}\sum_{i=1}^{N_x}\frac{(w^x_{i+1/2,jk})^2+(w^x_{i-1/2,jk})^2}{2}h_{x_i}\\
=&\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{y_j}h_{z_k}\Big(\sum_{i=2}^{N_x}\frac{h_{x,i-1/2}}{2}(w^x_{i-1/2,jk})^2+\sum_{i=1}^{N_x}\frac{h_{x_i}}{2}(w^x_{i-1/2,jk})^2\Big)\\
=&\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{y_j}h_{z_k}\sum_{i=2}^{N_x}\frac{h_{x,i-1/2}+h_{x_i}}{2}(w^x_{i-1/2,jk})^2\\
=&\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x,i-1/2}h_{y_j}h_{z_k}(w^x_{i-1/2,jk})^2,
\end{aligned}$$

we have $||\hat{w}^x||_m\le||w^x||_x$. The other two terms are proved in a similar manner. □

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

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

where M is a constant independent of q and h.

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

$$||w^x||_x\le||D_xw^x||_m,\quad ||w^y||_y\le||D_yw^y||_m,\quad ||w^z||_z\le||D_zw^z||_m. \tag{2.5}$$

Proof. $||w^x||_x\le||D_xw^x||_m$ is proved first. The other two inequalities are discussed similarly. From the fact that

$$w^x_{l+1/2,jk}=\sum_{i=1}^{l}\big(w^x_{i+1/2,jk}-w^x_{i-1/2,jk}\big)=\sum_{i=1}^{l}\frac{w^x_{i+1/2,jk}-w^x_{i-1/2,jk}}{h_{x_i}}h^{1/2}_{x_i}h^{1/2}_{x_i},$$

and by Cauchy inequality, we have

$$\big(w^x_{l+1/2,jk}\big)^2\le x_l\sum_{i=1}^{N_x}h_{x_i}\Big(\big[D_xw^x\big]_{ijk}\Big)^2.$$

Multiplying both sides by $h_{x,i+1/2}h_{y_j}h_{z_k}$ and making the summation, we have

$$\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}(w^x_{i-1/2,jk})^2h_{x,i-1/2}h_{y_j}h_{z_k}\le\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z}\Big(\big[D_xw^x\big]_{ijk}\Big)^2h_{x_i}h_{y_j}h_{z_k}.$$

Then the proof is completed. □

The mid-step partition is dynamical, obtained by refining the large-step partition of $\Omega=\{[0,1]\}^3$ uniformly. Generally, the mid-step is taken by 1/2 or 1/4 times the large-step, $h_{\hat{c}}=h_p/\hat{l}$ for $\hat{l}=2$ or $\hat{l}=4$. This local refined treatment is used and moves on t for the sharp fronts of the concentration and temperature. Other notation has the same definitions as above. The numbers of nodes in different directions, N_x, N_y and N_z are unchanged during the computations.

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

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

where M_1, M_2 and M_3 are positive constants. The space steps and other notation are denoted by $h^x=\frac{1}{M_1}$, $h^y=\frac{1}{M_2}$, $h^z=\frac{1}{M_3}$, $x_i=i\cdot h^x$, $y_j=j\cdot h^y$, $z_k=k\cdot h^z$ and $h_c=((h^x)^2+(h^y)^2+(h^z)^2)^{1/2}$. Let $D_{i+1/2,jk}=\frac{1}{2}[D(X_{ijk})+D(X_{i+1,jk})]$ and $D_{i-1/2,jk}=\frac{1}{2}[D(X_{ijk})+D(X_{i-1,jk})]$, 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. Let

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

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

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

and

$$\nabla_h(D\nabla W)^n_{ijk}=\delta_{\bar{x}}(D\delta_x W)^n_{ijk}+\delta_{\bar{y}}(D\delta_y W)^n_{ijk}+\delta_{\bar{z}}(D\delta_z W)^n_{ijk}. \tag{2.7}$$

3 An upwind mixed volume element-fractional step difference on a changing mesh

3.1 The procedures

The flow equation (1.1) is changed into a standard form

$$\phi_1\frac{\partial p}{\partial t}+\nabla\cdot\mathbf{u}=R(\hat{c}), \tag{3.1a}$$

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

where $R(\hat{c})=-q+R_s'$ and $a(\hat{c})=\kappa(X)\mu^{-1}(\hat{c})$.

The brine concentration equation (1.3) is rewritten in a divergent form to construct the computational scheme. Let $\mathbf{g}=\mathbf{u}\hat{c}=(u_1\hat{c},u_2\hat{c},u_3\hat{c})^T$, $\bar{\mathbf{z}}=-\nabla\hat{c}$ and $\mathbf{z}=E_c\bar{\mathbf{z}}$. Then,

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

Substituting $\nabla\cdot\mathbf{u}=-\phi\frac{\partial p}{\partial t}-q+R_s'(\hat{c})$ into (3.3),

$$\phi\frac{\partial\hat{c}}{\partial t}+\hat{c}\phi_1\frac{\partial p}{\partial t}+\nabla\cdot\mathbf{g}+\nabla\cdot\mathbf{z}=F(\hat{c}), \tag{3.3}$$

where $F(\hat{c})=-\hat{c}q+R_s'(\hat{c})+f(\hat{c})$.

The expanded mixed volume element [35] is adopted, then the flux $\mathbf{z}$ and its gradient $\bar{\mathbf{z}}$ can be computed simultaneously. The heat conduction equation (1.2) is discussed in a similar manner. Let $\mathbf{g}_T=c_p\mathbf{u}T=(u_1c_pT,u_2c_pT,u_3c_pT)^T$, $\bar{\mathbf{z}}_T=-\nabla T$ and $\mathbf{z}_T=E_H\bar{\mathbf{z}}_T$. Then,

$$d_{1,T}\frac{\partial p}{\partial t}+d_2\frac{\partial T}{\partial t}+\nabla\cdot\mathbf{g}_T+\nabla\cdot\mathbf{z}_T=Q_T(\mathbf{u},p,T,\hat{c}), \tag{3.4}$$

where $d_{1,T}=d_1(p)+c_p\phi_1T$ and $Q_T(\mathbf{u},p,T,\hat{c})=Q(\mathbf{u},p,T,\hat{c})-c_pqT+c_pTR_s'(\hat{c})$.

Let P, $\mathbf{U}$, $\hat{C}$, $\bar{\mathbf{Z}}$ and $\mathbf{Z}$ denote numerical solutions of p, $\mathbf{u}$, $\hat{c}$, $\bar{\mathbf{z}}$ and $\mathbf{z}$, respectively. Using Lemma 2.1-Lemma 2.4, we obtain the procedures of mixed volume element for the flow equation (3.1)

$$\begin{aligned}
&\Big(\phi_1\frac{P^{n+1}-P^n}{\Delta t},v\Big)_m+\big(D_xU^{x,n+1}+D_yU^{y,n+1}+D_zU^{z,n+1},v\big)_m\\
&=\big(R(\hat{C}^n),v\big)_m,\quad \forall v\in S_h, &(3.5a)\\
&\big(a^{-1}(\bar{\hat{C}}^{x,n})U^{x,n+1},w^x\big)_x+\big(a^{-1}(\bar{\hat{C}}^{y,n})U^{y,n+1},w^y\big)_y+\big(a^{-1}(\bar{\hat{C}}^{z,n})U^{z,n+1},w^z\big)_z\\
&-\big(P^{n+1},D_xw^x+D_xw^y+D_xw^z\big)_m=0,\quad \forall\mathbf{w}\in V_h. &(3.5b)
\end{aligned}$$

The upwind mixed volume element scheme on a changing mesh for Eq. (3.3) is defined by

$$\begin{aligned}
&\Big(\phi\frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t},v\Big)_m+\Big(\phi_1\hat{C}^n\frac{P^{n+1}-P^n}{\Delta t},v\Big)_m+\big(\nabla\cdot\mathbf{G}^{n+1},v\big)_m+\Big(\sum_{s=x,y,z}D_s\mathbf{Z}^{s,n+1},v\Big)_m\\
&=\big(F(\hat{C}^n),v\big)_m,\quad \forall v\in S_h, &(3.6a)\\
&\sum_{s=x,y,z}\big(\bar{Z}^{s,n+1},w^s\big)_s-\Big(\hat{C}^{n+1},\sum_{s=x,y,z}D_sw^s\Big)_m=0,\quad \forall\mathbf{w}\in V_h, &(3.6b)\\
&\sum_{s=x,y,z}\big(Z^{s,n+1},w^s\big)_s=\sum_{s=x,y,z}\big(E_c\bar{Z}^{s,n+1},w^s\big)_m,\quad \forall\mathbf{w}\in V_h. &(3.6c)
\end{aligned}$$

T_h, $\bar{\mathbf{Z}}_T$ and $\mathbf{Z}_T$ are numerical solutions of T, $\bar{\mathbf{z}}_T$ and $\mathbf{z}_T$. The computational scheme on a changing mesh is stated as follows for (3.4)

$$\begin{aligned}
&\Big(d_2\frac{T_h^{n+1}-T_h^n}{\Delta t},v\Big)_m+\Big(d_{1,T}(P^n,T_h^n)\frac{P^{n+1}-P^n}{\Delta t},v\Big)_m+\big(\nabla\cdot\mathbf{G}_T^{n+1},v\big)_m+\Big(\sum_{s=x,y,z}D_sZ_T^{s,n+1},v\Big)_m\\
&=\big(Q_T(\mathbf{U}^n,P^n,T_h^n,\hat{C}^n),v\big)_m,\quad \forall v\in S_h, &(3.7a)
\end{aligned}$$

$$\sum_{s=x,y,z}\left(\bar{Z}_T^{s,n+1},w^s\right)_s-\left(T_h^{n+1},\sum_{s=x,y,z}D_s w^s\right)_m=0,\quad \forall \mathbf{w}\in V_h, \tag{3.7b}$$

$$\sum_{s=x,y,z}\left(Z_T^{s,n+1},w^s\right)_s=\sum_{s=x,y,z}\left(E_H\bar{Z}_T^{s,n+1},w^s\right)_m,\quad \forall \mathbf{w}\in V_h. \tag{3.7c}$$

The radionuclide concentration (1.4) is solved by the following upwind fractional step difference scheme

$$\begin{aligned}\phi_{l,ijk}\frac{C_{l,ijk}^{n+1/3}-C_{l,ijk}^n}{\Delta t}=&\delta_{\bar{x}}(E_c\delta_x C_l^{n+1/3})_{ijk}+\delta_{\bar{y}}(E_c\delta_y C_l^n)_{ijk}+\delta_{\bar{z}}(E_c\delta_z C_l^n)_{ijk}-d_1(C_{ijk}^n)\frac{P_{ijk}^{n+1}-P_{ijk}^n}{\Delta t}\\&+f_l(\hat{C}^{n+1},C_1^n,C_2^n,\cdots,C_N^n)_{ijk}\\&-\sum_{s=x,y,z}\delta_{U_s^{n+1}}C_{l,ijk}^n,\quad 1\le i\le M_1,\quad l=1,2,\cdots,N,\end{aligned} \tag{3.8a}$$

$$\phi_{l,ijk}\frac{C_{l,ijk}^{n+2/3}-C_{l,ijk}^{n+1/3}}{\Delta t}=\delta_{\bar{y}}(E_c\delta_y(C_l^{n+2/3}-C_l^n))_{ijk},\quad 1\le j\le M_2,\quad l=1,2,\cdots,N, \tag{3.8b}$$

$$\phi_{l,ijk}\frac{C_{l,ijk}^{n+1}-C_{l,ijk}^{n+2/3}}{\Delta t}=\delta_{\bar{z}}(E_c\delta_z(C_l^{n+1}-C_l^n))_{ijk},\quad 1\le k\le M_3,\quad l=1,2,\cdots,N, \tag{3.8c}$$

where $\phi_l=\phi K_l$, $\delta_{U_s^{n+1}}C_{l,ijk}^n=U_{s,ijk}^{n+1}\{H(U_{s,ijk}^{n+1})\delta_{\bar{s}}C_{l,ijk}^n+(1-H(U_{s,ijk}^{n+1}))\delta_s C_{l,ijk}^n\}$.

Initial approximations:

$$P^0=\tilde{P}^0,\ \mathbf{U}^0=\tilde{\mathbf{U}}^0,\ \hat{C}^0=\tilde{\hat{C}}^0,\ \bar{\mathbf{Z}}^0=\tilde{\bar{\mathbf{Z}}}^0,\ \mathbf{Z}^0=\tilde{\mathbf{Z}}^0,\ T_h^0=\tilde{T}^0,\ \bar{\mathbf{Z}}_T^0=\tilde{\bar{\mathbf{Z}}}_T^0,\ \mathbf{Z}_T^0=\tilde{\mathbf{Z}}_T^0,\ X\in\Omega, \tag{3.9a}$$

$$C_{l,ijk}^0=\tilde{C}_{l0}(X_{ijk}),\quad X_{ijk}\in\bar{\Omega},\quad l=1,2,\cdots,N. \tag{3.9b}$$

Here $\{\tilde{P}^0,\tilde{\mathbf{U}}^0\}$, $\{\tilde{\hat{C}}^0,\tilde{\mathbf{Z}}^0,\tilde{\bar{\mathbf{Z}}}^0\}$ and $\{\tilde{T}_h^0,\tilde{\bar{\mathbf{Z}}}_T^0,\tilde{\mathbf{Z}}_T^0\}$ are obtained by using the Ritz projection for $\{p^0,\mathbf{u}^0\}$, $\{\hat{c}_0,\bar{\mathbf{z}}^0,\mathbf{z}_0\}$ and $\{T^0,\bar{\mathbf{z}}_T^0,\mathbf{z}_T^0\}$ (the definition of Ritz projection can be found in the following section). $\tilde{C}_{l,ijk}^0$ is defined by (1.6).

The upwind-term of (3.6a) is treated by a simple upwind approximation dependent on $\hat{C}$. Since $\mathbf{g}=\mathbf{u}c=0$ on $\partial\Omega$, we assign the mean value of the integral of $\mathbf{G}^{n+1}\cdot\mathbf{fl}$ 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. Define

$$\mathbf{G}^{n+1}\cdot\mathbf{fl}_l=\begin{cases}\hat{C}_{e_1}^{n+1}(\mathbf{U}^{n+1}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n+1}\cdot\gamma_l)(X_l)\ge 0,\\ \hat{C}_{e_2}^{n+1}(\mathbf{U}^{n+1}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n+1}\cdot\gamma_l)(X_l)<0.\end{cases} \tag{3.10}$$

$\hat{C}_{e_1}^{n+1}$ and $\hat{C}_{e_2}^{n+1}$ are the values of $\hat{C}^{n+1}$ on the elements. Then $\mathbf{G}^{n+1}$ is defined and the scheme of (3.6a)-(3.6c) is constructed. A nonsymmetric matrix is given to compute $\hat{C}$. If $\mathbf{G}^{n+1}$ is defined by the values at the previous time level, then a symmetric matrix is formed

$$\mathbf{G}^{n+1}\cdot\mathbf{fl}_l=\begin{cases}\hat{C}_{e_1}^{n}(\mathbf{U}^{n}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n}\cdot\gamma_l)(X_l)\ge 0,\\ \hat{C}_{e_2}^{n}(\mathbf{U}^{n}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n}\cdot\gamma_l)(X_l)<0.\end{cases} \tag{3.11}$$

Similarly, T_h is used to treat the convection term of (3.7a). Let $\mathbf{g}_T = c_p\mathbf{u}T = 0$ on $\partial\Omega$ and define

$$\mathbf{G}_T^{n+1}\cdot\mathbf{fl}_l = \begin{cases} c_p T_{h,e_1}^{n+1}(\mathbf{U}^{n+1}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n+1}\cdot\gamma_l)(X_l)\geq 0,\\ c_p T_{h,e_2}^{n+1}(\mathbf{U}^{n+1}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n+1}\cdot\gamma_l)(X_l)<0,\end{cases} \tag{3.12}$$

or

$$\mathbf{G}_T^{n+1}\cdot\mathbf{fl}_l = \begin{cases} c_p T_{h,e_1}^{n}(\mathbf{U}^{n}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n}\cdot\gamma_l)(X_l)\geq 0,\\ c_p T_{h,e_2}^{n}(\mathbf{U}^{n}\cdot\gamma_l)(X_l), & (\mathbf{U}^{n}\cdot\gamma_l)(X_l)<0.\end{cases} \tag{3.13}$$

The combined procedures run as follows. $\{\tilde{P}^0,\tilde{\mathbf{U}}^0\}$ and $\{\tilde{\hat{C}}^0,\tilde{\bar{\mathbf{Z}}}^0,\tilde{\mathbf{Z}}^0\}$ are determined by (1.6) and the Ritz projection, then initial approximations are given by $P^0=\tilde{P}^0$, $\mathbf{U}^0=\tilde{\mathbf{U}}^0$, $\hat{C}^0=\tilde{\hat{C}}^0$, $\bar{\mathbf{Z}}^0=\tilde{\bar{\mathbf{Z}}}^0$, $\mathbf{Z}^0=\tilde{\mathbf{Z}}^0$. Using (3.5) and the conjugate gradient method we find $\{P^1,\mathbf{U}^1\}$. Then, $\{\hat{C}^1,\bar{\mathbf{Z}}^1,\mathbf{Z}^1\}$ are obtained from (3.6) and the method of conjugate gradient. We apply (1.6) and the Ritz projection to determine $\{\tilde{T}_h^0,\tilde{\bar{\mathbf{Z}}}_T^0,\tilde{\mathbf{Z}}_T^0\}$ and approximate initial solutions of (1.2) by $T_h^0=\tilde{T}_h^0$, $\bar{\mathbf{Z}}_T^0=\tilde{\bar{\mathbf{Z}}}_T^0$ and $\mathbf{Z}_T^0=\tilde{\mathbf{Z}}_T^0$. Then $\{T_h^1,\bar{\mathbf{Z}}_T^0,\mathbf{Z}_T^1\}$ is computed by using the changing-mesh upwind mixed volume element scheme (3.7). Using the upwind fractional step difference scheme of (3.8a)-(3.8c) and the algorithm of speedup we get $\{C_{l,ijk}^{1/3}\}$ and $\{C_{l,ijk}^{2/3}\}$, then obtain $\{C_{l,ijk}^1\}$, the numerical solution at $t=t^1$. The concentrations are computed in parallel for $l=1,2,\cdots,N$. All the numerical solutions at $t=t^1$ are obtained. In a similar procession, we get $\{P^2,\mathbf{U}^2\}$, $\{\hat{C}^2,\bar{\mathbf{Z}}^2,\mathbf{Z}^2\}$, $\{T_h^2,\bar{\mathbf{Z}}_T^2,\mathbf{Z}_T^2\}$ and $\{C_l^2,l=1,2,\cdots,N\}$ from (3.5), (3.6), (3.7) and (3.8) in turns. When the approximate solutions at $t=t^{n-1}$ are given, we can obtain the numerical solutions at $t=t^n$ as above. They exist and are unique under the assumption (C).

Remark 3.1. Since the meshes are changing, $(\phi_1\hat{C}^n,v)_m$ in (3.6a) must be computed. That is, the L^2-projection of $\hat{C}^n$ is defined by a piecewise constant function on J_e^n mapping into a piecewise constant function on J_e^{n+1}. J_e^n and J_e^{n+1} denote different partition at t^n and t^{n+1}, respectively. $(d_2T_h^n,v)_m$ in (3.7b) is computed similarly.

4 The law of conservation

Suppose that the problem of (1.1)-(1.5) has slight compressibility [2,11,33,34], i.e., $\phi_1\cong 0$, and it has no source or sink, i.e., $F(\hat{c})\equiv 0$. Suppose that there is no permeation across the boundary, then on each element e of the unchanging mid-step partition, $e=\Omega_{ijk}=[x_{i-1/2},x_{i+1/2}]\times[y_{j-1/2},y_{j+1/2}]\times[z_{k-1/2},z_{k+1/2}]$, the concentration of brine has elemental conservation of mass

$$\int_e \phi\frac{\partial\hat{c}}{\partial t}dX - \int_{\partial e}\mathbf{g}\cdot\gamma_e ds - \int_{\partial e}\mathbf{z}\cdot\gamma_e ds = 0, \tag{4.1}$$

where ∂e is the boundary of e and γ_e is the outer normal vector. The following theorem shows that (3.6a) has the discrete form of (4.1).

Theorem 4.1. *If $\phi_1 \cong 0$ and $F(\hat{c}) \equiv 0$ hold, then* (3.6a) *has the elemental conservation of mass for numerical solutions on $e \in \Omega$*

$$\int_e \phi \frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t} dX - \int_{\partial e} \mathbf{G}^{n+1} \cdot \gamma_e ds - \int_{\partial e} \mathbf{Z}^{n+1} \cdot \gamma_e ds = 0. \tag{4.2}$$

Proof. For $v \in S_h$, let

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

then (3.6a) is changed into

$$\Big(\phi \frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t}, 1\Big)_{\Omega_{ijk}} - \int_{\partial \Omega_{ijk}} \mathbf{G}^{n+1} \cdot \gamma_{\Omega_{ijk}} ds + \Big(\sum_{s=x,y,z} D_s Z^{s,n+1}, 1\Big)_{\Omega_{ijk}} = 0. \tag{4.3}$$

Using the notations in Section 2, we have

$$\Big(\phi \frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t}, 1\Big)_{\Omega_{ijk}} = \phi_{ijk} \Big(\frac{\hat{C}^{n+1}_{ijk}-\hat{C}^n_{ijk}}{\Delta t}\Big) h_{x_i} h_{y_j} h_{z_k} = \int_{\Omega_{ijk}} \phi \frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t} dX, \tag{4.4a}$$

$$\begin{aligned}\Big(\sum_{s=x,y,z} D_s Z^{s,n+1}, 1\Big)_{\Omega_{ijk}} =& \Big(Z^{x,n+1}_{i+1/2,jk} - Z^{x,n+1}_{i-1/2,jk}\Big) h_{y_j} h_{z_k} + \Big(Z^{y,n+1}_{i,j+1/2,k} - Z^{y,n+1}_{i,j-1/2,k}\Big) h_{x_i} h_{z_k} \\ &+ \Big(Z^{z,n+1}_{ij,k+1/2} - Z^{z,n+1}_{ij,k-1/2}\Big) h_{x_i} h_{y_j} = -\int_{\partial \Omega_{ijk}} \mathbf{Z}^{n+1} \cdot \gamma_{\Omega_{ijk}} ds. \end{aligned}\tag{4.4b}$$

Substituting (4.4) into (4.3), we complete the proof. □

Then the whole conservation of mass is derived as follow.

Theorem 4.2. *If $\phi_1 \cong 0$, $F(\hat{c}) \equiv 0$ and the impermeable boundary condition hold, then* (3.6a) *has the conservation of mass on the whole domain*

$$\int_\Omega \phi \frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t} dX = 0, \quad n \geq 0. \tag{4.5}$$

Proof. Summing (4.2) on all the elements, we have

$$\sum_{i,j,k} \int_{\Omega_{ijk}} \phi \frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t} dX - \sum_{i,j,k} \int_{\partial \Omega_{ijk}} \mathbf{G}^{n+1} \cdot \gamma_{\Omega_{ijk}} ds - \sum_{i,j,k} \int_{\partial \Omega_{ijk}} \mathbf{Z}^{n+1} \cdot \gamma_{\Omega_{ijk}} ds = 0. \tag{4.6}$$

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 $\mathbf{U}^{n+1} \cdot \gamma_l(X_l) \geq 0$ on e_1, then

$$\int_{e_1} \mathbf{G}^{n+1} \cdot \gamma_l ds = \hat{C}^{n+1}_{e_1} \mathbf{U}^{n+1} \cdot \gamma_l(X_l) |\sigma_l|. \tag{4.7a}$$

Here $|\sigma_l|$ denotes the measure of σ_l. The outer normal vector on e_2 is $-\gamma_l$, so $\mathbf{U}^{n+1}\cdot\gamma_l(X_l)\leq 0$. Then,

$$\int_{e_2}\mathbf{G}^{n+1}\cdot\gamma_l ds=-\hat{C}_{e_1}^{n+1}\mathbf{U}^{n+1}\cdot\gamma_l(X_l)|\sigma_l|. \tag{4.7b}$$

Since (4.7b) is opposite to (4.7a), so we have

$$\sum_e\int_{\partial e}\mathbf{G}^{n+1}\cdot\gamma_{\partial e}ds=0. \tag{4.8}$$

Combing the following fact

$$-\sum_e\int_{\partial e}\mathbf{Z}^{n+1}\cdot\gamma_{\partial e}ds=-\int_{\partial\Omega}\mathbf{Z}^{n+1}\cdot\gamma_{\partial\Omega}ds=0, \tag{4.9}$$

and substituting (4.7) and (4.8) into (4.6), we obtain (4.5) and complete the proof. □

Suppose that Eq. (1.2) has three conditions: 1) slight compressibility, i.e., $d_{1,T}\cong 0$, 2) no source or sink, 3) impermeable boundary. Then (3.4) has the elemental conservation of energy. Similar to the discussions of Theorem 4.1 and Theorem 4.2, we can obtain the discrete conservation of energy on every element and on the whole domain for (3.7a).

Theorem 4.3. *If $d_{1,T}\cong 0$ and $Q_T\equiv 0$ hold, then* (3.7a) *has the elemental conservative nature on e,*

$$\int_e d_2\frac{T_h^{n+1}-T_h^n}{\Delta t}dX-\int_{\partial e}\mathbf{G}^{n+1}\cdot\gamma_e ds-\int_{\partial e}\mathbf{Z}^{n+1}\cdot\gamma_e ds=0. \tag{4.10}$$

Theorem 4.4. *If $d_{1,T}\cong 0$ and $Q_T\equiv 0$ hold, and no heat conducts through the boundary, then* (3.7a) *has the whole conservation of energy*

$$\int_\Omega\phi\frac{T_h^{n+1}-T_h^n}{\Delta t}dX=0,\quad n\geq 0. \tag{4.11}$$

The nature of conservation is an important physical standard in numerical simulation of seepage mechanics.

5 Convergence analysis

First we introduce a Ritz projection to determine initial approximations. Define $\{\tilde{P},\tilde{\mathbf{U}}\}\in S_h\times V_h$ by

$$\Big(\sum_{s=x,y,z}D_s\tilde{U}^s,v\Big)_m=(f,v)_m,\quad\forall v\in S_h, \tag{5.1a}$$

$$\sum_{s=x,y,z}\big(a^{-1}(\hat{c})\tilde{U}^s,w^s\big)_s=\Big(\tilde{P},\sum_{s=x,y,z}D_sw^s\Big)_m,\quad\forall\mathbf{w}\in V_h, \tag{5.1b}$$

$$\big(\tilde{P}-p,1\big)_m=0, \tag{5.1c}$$

where $f=-\phi\frac{\partial p}{\partial t}-q+R_s'(\hat{c})$.

Define $\{\tilde{\hat{C}},\tilde{\bar{\mathbf{Z}}},\tilde{\mathbf{Z}}\}\in S_h\times V_h\times V_h$ by

$$\Big(\sum_{s=x,y,z} D_s\tilde{Z}^s,v\Big)_m=\big(f_{\hat{c}},v\big)_m,\quad \forall v\in S_h, \tag{5.2a}$$

$$\Big(\sum_{s=x,y,z} \tilde{\bar{Z}}^s,w^s\Big)_s=\Big(\tilde{\hat{C}},\sum_{s=x,y,z} D_s w^s\Big)_m,\quad \forall \mathbf{w}\in V_h, \tag{5.2b}$$

$$\sum_{s=x,y,z}\big(\tilde{Z}^s,w^s\big)_s=\sum_{s=x,y,z}\big(E_c\tilde{\bar{Z}}^s,w^s\big)_s,\quad \forall \mathbf{w}\in V_h, \tag{5.2c}$$

$$\big(\tilde{\hat{C}}-\hat{c},1\big)_m=0, \tag{5.2d}$$

where $f_{\hat{c}}=-\phi\frac{\partial \hat{c}}{\partial t}-\mathbf{u}\cdot\nabla\hat{c}+f(\hat{c})$.

Define $\{\tilde{T}_h,\tilde{\bar{\mathbf{Z}}}_T,\tilde{\mathbf{Z}}_T\}\in S_h\times V_h\times V_h$ by

$$\Big(\sum_{s=x,y,z} D_s\tilde{Z}_T^s,v\Big)_m=\big(f_T,v\big)_m,\quad \forall v\in S_h, \tag{5.3a}$$

$$\Big(\sum_{s=x,y,z} \tilde{\bar{Z}}_T^s,w^s\Big)_s=\Big(\tilde{T}_h,\sum_{s=x,y,z} D_s w^s\Big)_m,\quad \forall \mathbf{w}\in V_h, \tag{5.3b}$$

$$\sum_{s=x,y,z}\big(\tilde{Z}_T^s,w^s\big)_s=\sum_{s=x,y,z}\big(E_H\tilde{\bar{Z}}_T^s,w^s\big)_s,\quad \forall \mathbf{w}\in V_h, \tag{5.3c}$$

$$\big(\tilde{T}_h-T,1\big)_m=0, \tag{5.3d}$$

where $f_T=-d_1(p)\frac{\partial p}{\partial t}-d_2\frac{\partial T}{\partial t}-c_p\mathbf{u}\cdot\nabla T+Q$.

Let $\pi=P-\tilde{P}$, $\eta=\tilde{P}-p$, $\boldsymbol{\sigma}=\mathbf{U}-\tilde{\mathbf{U}}$, $\boldsymbol{\rho}=\tilde{\mathbf{U}}-\mathbf{u}$, $\xi_{\hat{c}}=\hat{C}-\tilde{\hat{C}}$, $\zeta_{\hat{c}}=\tilde{\hat{C}}-\hat{c}$, $\bar{\alpha}_{\hat{c}}=\bar{\mathbf{Z}}-\tilde{\bar{\mathbf{Z}}}$, $\bar{\beta}_{\hat{c}}=\tilde{\bar{\mathbf{Z}}}-\bar{\mathbf{z}}$, $\alpha_c=\mathbf{Z}-\tilde{\mathbf{Z}}$, $\beta_c=\tilde{\mathbf{Z}}-\mathbf{z}$, $\xi_T=T_h-\tilde{T}_h$, $\zeta_T=\tilde{T}_h-T$, $\bar{\alpha}_T=\bar{\mathbf{Z}}_T-\tilde{\bar{\mathbf{Z}}}_T$, $\bar{\beta}_T=\tilde{\bar{\mathbf{Z}}}_T-\bar{\mathbf{z}}_T$, $\alpha_T=\mathbf{Z}_T-\tilde{\mathbf{Z}}_T$ and $\beta_T=\tilde{\mathbf{Z}}_T-\mathbf{z}_T$. The problem of (1.1)-(1.6) is supposed to be positive definite and regular. From the discussions of Weiser, Wheeler [24] and Arbogast, Wheeler, Yotov [35], it is easy to see that the auxiliary solutions $\{\tilde{P},\tilde{\mathbf{U}},\tilde{\hat{C}},\tilde{\bar{Z}},\tilde{\mathbf{Z}}\}$ and $\{\tilde{T}_h,\tilde{\bar{\mathbf{Z}}}_T,\tilde{\mathbf{Z}}_T\}$ of (5.1)-(5.3) exist and are unique.

Lemma 5.1. *The coefficients and exact solutions of* (1.1)-(1.6) *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*

$$\begin{aligned}&||\eta||_m+\sum_{s=\hat{c},T}||\zeta_s||_m+|||\text{æ}|||+\sum_{s=\hat{c},T}[|||\bar{\mathbf{fi}}|||+|||\beta_s|||]+\Big|\Big|\frac{\partial\eta}{\partial t}\Big|\Big|_m+\sum_{s=\hat{c},T}\Big|\Big|\frac{\partial\zeta_s}{\partial t}\Big|\Big|_m\\&\le\bar{C}_1\{h_p^2+h_{\hat{c}}^2\},\end{aligned} \tag{5.4a}$$

$$|||\tilde{\mathbf{U}}|||_\infty+\sum_{s=\hat{c},T}\Big[|||\tilde{\bar{\mathbf{Z}}}_s|||_\infty+|||\tilde{\mathbf{Z}}_s|||_\infty\Big]\le\bar{C}_2. \tag{5.4b}$$

In this paper we show convergence analysis for a model problem. Let $\mu(\hat{c})\approx\mu_0$, $a(\hat{c})=\kappa(X)\mu^{-1}(\hat{c})\approx\kappa(X)\mu_0^{-1}=a(X)$ and $R_s'\equiv 0$ in (1.1) and (1.3). This assumption is reasonable for the mixture fluid with "slight compressibility" [3, 36]. The problem is simplified into

$$\phi_1 \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{u} = R(\hat{c}), \quad X \in \Omega, \quad t \in J, \tag{5.5a}$$

$$\mathbf{u} = -a \nabla p, \quad X \in \Omega, \quad t \in J, \tag{5.5b}$$

and

$$\phi \frac{\partial \hat{c}}{\partial t} + \mathbf{u} \cdot \nabla \hat{c} - \nabla \cdot (E_c \nabla \hat{c}) = f(\hat{c}), \quad X \in \Omega, \quad t \in J. \tag{5.6}$$

The mixed volume element scheme of (3.5) is simplified into

$$\begin{aligned}
&\Big(\phi_1 \frac{P^{n+1} - P^n}{\Delta t}, v\Big)_m + \big(D_x U^{x,n+1} + D_y U^{y,n+1} + D_z U^{z,n+1}, v\big)_m \\
&= \big(R(\hat{C}^n), v\big)_m, \quad \forall v \in S_h, \qquad (5.7a)\\
&\big(a^{-1} U^{x,n+1}, w^x\big)_x + \big(a^{-1} U^{y,n+1}, w^y\big)_y + \big(a^{-1} U^{z,n+1}, w^z\big)_z - \big(P^{n+1}, D_x w^x + D_x w^y + D_x w^z\big)_m \\
&= 0, \quad \forall \mathbf{w} \in V_h. \qquad (5.7b)
\end{aligned}$$

We estimate π and σ first. By subtracting (5.1a) ($t = t^{n+1}$) and (5.1b) ($t = t^{n+1}$), respectively, from (3.5a) and (3.5b), we obtain

$$\begin{aligned}
&\big(\phi_1 \partial_t \pi^n, v\big)_m + \big(D_x \sigma^{x,n+1} + D_y \sigma^{y,n+1} + D_z \sigma^{z,n+1}, v\big)_m \\
&= -\Big(\phi_1 \Big(\partial_t \tilde{P}^n - \frac{\partial \tilde{p}^{n+1}}{\partial t}\Big), v\Big)_m - \big(\phi_1 \partial_t \eta^n, v\big)_m + \big(R(\hat{C}^n) - R(\hat{c}^{n+1}), v\big)_m, \quad \forall v \in S_h, \qquad (5.8a)\\
&\big(a^{-1} \sigma^{x,n+1}, w^x\big)_x + \big(a^{-1} \sigma^{y,n+1}, w^y\big)_y + \big(a^{-1} \sigma^{z,n+1}, w^z\big)_z - \big(\pi^{n+1}, D_x w^x + D_y w^y + D_z w^z\big)_m \\
&= 0, \quad \forall \mathbf{w} \in V_h, \qquad (5.8b)
\end{aligned}$$

where $\partial_t \pi^n = (\pi^{n+1} - \pi^n)/\Delta t$, $\partial_t \tilde{P}^n = (\tilde{P}^{n+1} - \tilde{P}^n)/\Delta t$.

Taking $v = \partial_t \pi^n$ in (5.8a), dividing the difference of (5.8b) at t^{n+1} and t^n by Δt, taking $\mathbf{w} = \sigma^{n+1}$ then summing the results, and noting that for $A \geq 0$,

$$\begin{aligned}
\big(\partial_t (AB^n), B^{n+1}\big)_s &= \frac{1}{2} \partial_t \big(AB^n, B^n\big)_s + \frac{1}{2\Delta t} \big(A(B^{n+1} - B^n), B^{n+1} - B^n\big)_s \\
&\geq \frac{1}{2} \partial_t \big(AB^n, B^n\big)_s, \quad s = x, y, z,
\end{aligned}$$

we have

$$\begin{aligned}
&\big(\phi_1 \partial_t \pi^n, \partial_t \pi^n\big)_m + \frac{1}{2} \partial_t \Big[\big(a^{-1} \sigma^{x,n}, \sigma^{x,n}\big)_x + \big(a^{-1} \sigma^{y,n}, \sigma^{y,n}\big)_y + \big(a^{-1} \sigma^{z,n}, \sigma^{z,n}\big)_z\Big] \\
\leq & -\Big(\phi_1 \Big(\partial_t \tilde{P}^n - \frac{\partial \tilde{p}^{n+1}}{\partial t}\Big), \partial_t \pi^n\Big)_m - \Big(\phi_1 \frac{\partial \eta^{n+1}}{\partial t}, \partial_t \pi^n\Big)_m + \big(R(\hat{C}^n) - R(\hat{c}^{n+1}), \partial_t \pi^n\big)_m. \qquad (5.9)
\end{aligned}$$

By the positive definite condition (C) and Lemma 5.1,

$$\big(\phi_1\partial_t\pi^n,\partial_t\pi^n\big)_m\geq\phi_*\big|\big|\partial_t\pi^n\big|\big|_m^2, \tag{5.10a}$$

$$\begin{aligned}&-\Big(\phi_1\Big(\partial_t\tilde{P}^n-\frac{\partial\tilde{p}^{n+1}}{\partial t}\Big),\partial_t\pi^n\Big)_m-\Big(\phi_1\frac{\partial\eta^{n+1}}{\partial t},\partial_t\pi^n\Big)_m+\big(R(\hat{C}^n)-R(\hat{c}^{n+1}),\partial_t\pi^n\big)_m\\&\leq\varepsilon\big|\big|\partial_t\pi^n\big|\big|_m^2+K\big\{\big|\big|\xi_{\hat{c}}^n\big|\big|_m^2+h_p^4+h_{\hat{c}}^4+(\Delta t)^2\big\}.\end{aligned} \tag{5.10b}$$

Applying (5.10), we have

$$\big|\big|\partial_t\pi^n\big|\big|_m^2+\partial_t\sum_{s=x,y,z}\big(a^{-1}\sigma^{s,n},\sigma^{s,n}\big)_s\leq K\big\{\big|\big|\xi_{\hat{c}}^n\big|\big|_m^2+h_p^4+h_{\hat{c}}^4+(\Delta t)^2\big\}. \tag{5.11}$$

The concentration of brine (1.3) is discussed. Subtracting (5.2a), (5.2b) and (5.2c) at $t=t^{n+1}$ from (3.6a), (3.6b) and (3.6c), respectively, and taking $v=\xi_{\hat{c}}^{n+1}$, $\mathbf{w}=\alpha_{\hat{c}}^{n+1}$ and $\mathbf{w}=\bar{\alpha}_{\hat{c}}^{n+1}$ in the three differences, we have

$$\begin{aligned}&\Big(\phi\frac{\hat{C}^{n+1}-\hat{C}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m+\Big(\phi_1\hat{C}^n\frac{P^{n+1}-P^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m+\big(\nabla\cdot\mathbf{G}^{n+1},\xi_{\hat{c}}^{n+1}\big)_m+\Big(\sum_{s=x,y,z}D_s\alpha_{\hat{c}}^{s,n+1},\xi_{\hat{c}}^{n+1}\Big)_m\\&=\Big(F(\hat{C}^n)-F(\hat{c}^{n+1})+\phi\frac{\partial\hat{c}^{n+1}}{\partial t}+\phi\hat{c}^{n+1}\frac{\partial p^{n+1}}{\partial t}+\nabla\cdot\mathbf{g}^{n+1},\xi_{\hat{c}}^{n+1}\Big)_m,\end{aligned} \tag{5.12a}$$

$$\sum_{s=x,y,z}\big(\bar{\alpha}_{\hat{c}}^{s,n+1},\alpha_{\hat{c}}^{s,n+1}\big)_s=\Big(\xi_{\hat{c}}^{n+1},\sum_{s=x,y,z}D_s\alpha_{\hat{c}}^{s,n+1}\Big)_m, \tag{5.12b}$$

$$\sum_{s=x,y,z}\big(Z^{s,n+1},\bar{\alpha}_{\hat{c}}^{s,n+1}\big)_s=\sum_{s=x,y,z}\big(E_c\bar{Z}^{s,n+1},\bar{\alpha}_{\hat{c}}^{s,n+1}\big)_m. \tag{5.12c}$$

Subtracting (5.12c) from the sum of (5.12a) and (5.12b), we have

$$\begin{aligned}&\Big(\phi\frac{\xi_{\hat{c}}^{n+1}-\xi_{\hat{c}}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m+\big(\nabla\cdot\big(\mathbf{G}^{n+1}-\mathbf{g}^{n+1}\big),\xi_{\hat{c}}^{n+1}\big)_m\\&=\big(F(\hat{C}^n)-F(\hat{c}^{n+1}),\xi_{\hat{c}}^{n+1}\big)_m-\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m+\Big(\phi\Big(\frac{\partial\hat{c}^{n+1}}{\partial t}-\frac{\hat{c}^{n+1}-\hat{c}^n}{\Delta t}\Big),\xi_{\hat{c}}^{n+1}\Big)_m\\&\quad+\Big(\hat{c}^{n+1}\phi\frac{\partial p^{n+1}}{\partial t}-\hat{C}^n\phi\frac{P^{n+1}-P^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)-\sum_{s=x,y,z}\big(E_c\bar{\alpha}_{\hat{c}}^{s,n+1},\bar{\alpha}_{\hat{c}}^{s,n+1}\big)_m.\end{aligned} \tag{5.13}$$

Rewrite the above equation,

$$\begin{aligned}&\Big(\phi\frac{\xi_{\hat{c}}^{n+1}-\xi_{\hat{c}}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m+\sum_{s=x,y,z}\big(E_c\bar{\alpha}_{\hat{c}}^{s,n+1},\bar{\alpha}_{\hat{c}}^{s,n+1}\big)_m\\&=-\big(\nabla\cdot\big(\mathbf{G}^{n+1}-\mathbf{g}^{n+1}\big),\xi_{\hat{c}}^{n+1}\big)_m+\big(F(\hat{C}^n)-F(\hat{c}^{n+1}),\xi_{\hat{c}}^{n+1}\big)_m+\Big(\phi\Big(\frac{\partial\hat{c}^{n+1}}{\partial t}-\frac{\hat{c}^{n+1}-\hat{c}^n}{\Delta t}\Big),\xi_{\hat{c}}^{n+1}\Big)_m\\&\quad+\Big(\hat{c}^{n+1}\phi\frac{\partial p^{n+1}}{\partial t}-\hat{C}^n\phi\frac{P^{n+1}-P^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)-\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\\&=T_1+T_2+T_3+T_4+T_5.\end{aligned} \tag{5.14}$$

The left-hand side is estimated first,

$$\Big(\phi\frac{\xi_{\hat{c}}^{n+1}-\xi_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m \geq \frac{1}{2\Delta t}\Big\{\big(\phi\xi_{\hat{c}}^{n+1},\xi_{\hat{c}}^{n+1}\big)_m-\big(\phi\xi_{\hat{c}}^{n},\xi_{\hat{c}}^{n}\big)_m\Big\}, \tag{5.15a}$$

$$\sum_{s=x,y,z}\big(E_c\bar{\alpha}_{\hat{c}}^{s,n+1},\bar{\alpha}_{\hat{c}}^{s,n+1}\big)_m \geq E_*|||\bar{\alpha}_{\hat{c}}^{n+1}|||^2. \tag{5.15b}$$

The first term on the right-hand side of (5.14) is considered,

$$\begin{aligned}
&-\big(\nabla\cdot\big(\mathbf{G}^{n+1}-\mathbf{g}^{n+1}\big),\xi_{\hat{c}}^{n+1}\big)_m\\
=&\big(\big(\mathbf{G}^{n+1}-\mathbf{g}^{n+1}\big),\nabla\xi_{\hat{c}}^{n+1}\big)_m\\
\leq&\varepsilon|||\bar{\alpha}_{\hat{c}}^{n+1}|||^2+||\mathbf{G}^{n+1}-\mathbf{g}^{n}||_m^2.
\end{aligned} \tag{5.16}$$

Let σ denote the interface. γ_l is the outer normal vector and X_l is the barycenter. Then

$$\int_\sigma \mathbf{g}^{n+1}\cdot\gamma_l=\int_\sigma \hat{c}^{n+1}(\mathbf{u}^{n+1}\cdot\gamma_l)ds. \tag{5.17a}$$

By using the regularity of $\mathbf{g}^{n+1}$ and the mean value of integral, we have

$$\frac{1}{\mathrm{mes}(\sigma)}\int_\sigma(\mathbf{G}^{n+1}-\mathbf{g}^{n})\cdot\gamma_l=\hat{C}_e^{n+1}\big(\mathbf{U}^{n+1}\cdot\gamma_l\big)(X_l)-\big(\hat{c}^{n+1}\mathbf{u}^{n+1}\cdot\gamma_l\big)(X_l)+\mathcal{O}(h_{\hat{c}}), \tag{5.17b}$$

From the regularity of $\hat{c}^{n+1}$, Lemma 2.4 and the argument in [35],

$$\big|\hat{C}_e^{n+1}-\hat{c}^{n+1}(X_l)\big|\leq\big|\xi_{\hat{c}}^{n+1}\big|+\mathcal{O}(h_{\hat{c}}), \tag{5.18a}$$

$$\big|\mathbf{U}^{n+1}-\mathbf{u}^{n+1}\big|\leq\big|\xi_{\hat{c}}^{n+1}\big|+\mathcal{O}(h_{\hat{c}}). \tag{5.18b}$$

Continue,

$$||\mathbf{G}^{n+1}-\mathbf{g}^{n}||_m^2\leq K\Big\{||\xi_{\hat{c}}^{n+1}||_m^2+h_{\hat{c}}^2\Big\}. \tag{5.19}$$

The right-hand side terms of (5.14) are estimated as follows

$$|T_1|\leq\varepsilon|||\bar{\alpha}_{\hat{c}}^{n+1}|||^2+K\Big\{||\xi_{\hat{c}}^{n+1}||_m^2+h_{\hat{c}}^2\Big\}, \tag{5.20a}$$

$$|T_2|\leq K\Big\{||\xi_{\hat{c}}^{n}||_m^2+(\Delta t)^2+h_{\hat{c}}^4\Big\}, \tag{5.20b}$$

$$|T_3|\leq K\Big\{\Delta t||\frac{\partial^2\hat{c}}{\partial t^2}||_{L^2(t^n,t^{n+1};m)}^2+||\xi_{\hat{c}}^{n+1}||_m^2\Big\}, \tag{5.20c}$$

$$|T_4|\leq\varepsilon|\partial_t\pi^n||_m^2+K\Big\{\Delta t||\frac{\partial p}{\partial t}||_{L^2(t^n,t^{n+1};m)}^2+||\xi_{\hat{c}}^{n+1}||_m^2+||\xi_{\hat{c}}^{n}||_m^2+(\Delta t)^2\Big\}. \tag{5.20d}$$

Substituting (5.15) and (5.20) into (5.14),

$$\begin{aligned}&\frac{1}{2\Delta t}\Big\{||\phi^{1/2}\xi_{\hat{c}}^{n+1}||_m^2-||\phi^{1/2}\xi_{\hat{c}}^{n}||_m^2\Big\}+\frac{E_*}{2}|||\bar{\alpha}_{\hat{c}}^{n+1}|||^2\\ \leq& K||\frac{\partial p}{\partial t}||^2_{L^2(t^n,t^{n+1};m)}\Delta t+K\Big\{||\xi_{\hat{c}}^{n+1}||_m^2+||\xi_{\hat{c}}^{n}||_m^2+h_{\hat{c}}^2+(\Delta t)^2\Big\}+\varepsilon||\partial_t\pi^n||_m^2\\ &-\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m. \end{aligned}\tag{5.21}$$

Multiplying both sides of (5.21) by $2\Delta t$, summing them on n $(0\leq n\leq L-1)$ and using $\xi_{\hat{c}}^0=0$, we obtain

$$\begin{aligned}&||\phi^{1/2}\xi_{\hat{c}}^{L}||_m^2+\sum_{n=0}^{L}|||\bar{\alpha}_{\hat{c}}^{n}|||^2\Delta t\\ \leq& K\Big\{h_{\hat{c}}^2+(\Delta t)^2\Big\}+K\sum_{n=0}^{L}||\xi_{\hat{c}}^{n}||_m^2\Delta t+\varepsilon\sum_{n=0}^{L-1}|\partial_t\pi^n||_m^2\Delta t-2\sum_{n=0}^{L-1}\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\Delta t. \end{aligned}\tag{5.22}$$

The last term on the right-hand side of (5.22) is divided into two cases: changing mesh and unchanging mesh,

$$\begin{aligned}&-2\sum_{n=0}^{L-1}\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\Delta t\\ =&-2\sum_{n=n'}\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\Delta t-2\sum_{n=n''}\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\Delta t. \end{aligned}\tag{5.23}$$

$n=n'$ denotes the unchanging mesh,

$$-2\sum_{n=n'}\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\Delta t\leq Kh_{\hat{c}}^4+\varepsilon\sum_{n=0}^{L}||\xi_{\hat{c}}^{n+1}||^2\Delta t. \tag{5.23b}$$

$n=n''$ denotes the changing mesh,

$$\big(\phi\zeta_{\hat{c}}^{n''},\xi_{\hat{c}}^{n''}\big)_m=0. \tag{5.23c}$$

Suppose that the mesh changes at most $\bar{M}$ times, $\bar{M}\leq M^*$, where $\bar{M}$ is a positive integer independent of h and Δt. From (5.23) and Lemma 5.1,

$$-2\sum_{n=0}^{L-1}\Big(\phi\frac{\zeta_{\hat{c}}^{n+1}-\zeta_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\Delta t\leq K\big(M^*h_{\hat{c}}\big)^2+Kh_{\hat{c}}^4+\frac{1}{4}||\phi^{1/2}\xi_{\hat{c}}^{L}||^2+\varepsilon\sum_{n=0}^{L}||\xi_{\hat{c}}^{n}||^2\Delta t. \tag{5.24}$$

Substituting (5.24) into (5.22), we have

$$\begin{aligned}&||\phi^{1/2}\xi_{\hat{c}}^{L}||_m^2+\sum_{n=0}^{L}|||\bar{\alpha}^{n}|||^2\Delta t_c\\ \leq& K\big\{h_p^4+h_{\hat{c}}^2+\big(M^*h_{\hat{c}}\big)^2+(\Delta t)^2\big\}+K\sum_{n=0}^{L-1}||\xi_{\hat{c}}^{n+1}||^2\Delta t+\varepsilon\sum_{n=0}^{L-1}||\partial_t\pi^n||^2\Delta t. \end{aligned}\tag{5.25}$$

Multiplying both sides of (5.11) by Δt, summing them on n $(0\le n\le L-1)$ and using $\sigma^0=0$, we obtain

$$|||\sigma^L|||^2+\sum_{n=0}^{L-1}||\partial_t\pi^n||_m^2\Delta t\le K\Big\{\sum_{n=0}^{L}||\xi_{\hat c}^n||_m^2\Delta t+h_p^4+h_{\hat c}^4+(\Delta t)^2\Big\}. \tag{5.26}$$

Combining (5.22) and (5.26),

$$\begin{aligned}&|||\sigma^L|||^2+\sum_{n=0}^{L-1}||\partial_t\pi^n||_m^2\Delta t+||\xi_{\hat c}^L||_m^2+\sum_{n=0}^{L}|||\bar\alpha_{\hat c}^{n+1}|||^2\Delta t\\ \le& K\Big\{\sum_{n=0}^{L}||\xi_{\hat c}^n||_m^2\Delta t+h_p^4+h_{\hat c}^2+\big(M^*h_{\hat c}\big)^2+(\Delta t)^2\Big\}.\end{aligned} \tag{5.27}$$

Applying the discrete Gronwall's Lemma

$$\begin{aligned}&|||\sigma^L|||^2+\sum_{n=0}^{L-1}||\partial_t\pi^n||_m^2\Delta t+||\xi_{\hat c}^L||_m^2+\sum_{n=0}^{L}|||\bar\alpha_{\hat c}^{n+1}|||^2\Delta t\\ \le& K\Big\{h_p^4+h_{\hat c}^2+\big(M^*h_{\hat c}\big)^2+(\Delta t)^2\Big\}.\end{aligned} \tag{5.28}$$

A duality method is introduced to address $\pi^L\in S_h$ [37,38]. Consider the following elliptic problem,

$$\nabla\cdot\omega=\pi^L,\quad X=(x,y,z)^T\in\Omega, \tag{5.29a}$$
$$\omega=\nabla p,\quad X\in\Omega, \tag{5.29b}$$
$$\omega\cdot\gamma=0,\quad X\in\partial\Omega. \tag{5.29c}$$

It follows from the regularity that

$$\sum_{s=x,y,z}\Big|\Big|\frac{\partial\omega^s}{\partial s}\Big|\Big|^2\le M\Big|\Big|\pi^L\Big|\Big|^2. \tag{5.30}$$

Suppose that $\tilde\omega\in V_h$ is defined by

$$\Big(\frac{\partial\tilde\omega^s}{\partial s},v\Big)_m=\Big(\frac{\partial\omega^s}{\partial s},v\Big)_m,\quad \forall v\in S_h,\quad s=x,y,z. \tag{5.31a}$$

The solution $\tilde\omega$ exists and satisfies

$$\sum_{s=x,y,z}\Big|\Big|\frac{\partial\tilde\omega^s}{\partial s}\Big|\Big|_m^2\le\sum_{s=x,y,z}\Big|\Big|\frac{\partial\omega^s}{\partial s}\Big|\Big|_m^2. \tag{5.31b}$$

By Lemma 2.4, (5.29), (5.30) and (5.1), we have

$$\begin{aligned}||\pi^L||^2&=\big(\pi^L,\nabla\cdot\omega\big)=\big(\pi^L,\sum_{s=x,y,z}D_s\tilde\omega^s\big)_m=\sum_{s=x,y,z}\big(a^{-1}\sigma^{s,L},\tilde\omega^s\big)_s\\ &\le K|||\tilde\omega|||\cdot|||\sigma^L|||.\end{aligned} \tag{5.32}$$

Using Lemma 2.4, (5.30) and (5.31), we have

$$|||\tilde{\omega}|||^2 \leq \sum_{s=x,y,z} ||D_s\tilde{\omega}^s||_m^2 = \sum_{s=x,y,z} \Big|\Big|\frac{\partial\tilde{\omega}^s}{\partial s}\Big|\Big|_m^2 \leq \sum_{s=x,y,z} \Big|\Big|\frac{\partial\omega^s}{\partial s}\Big|\Big|_m^2 \leq K||\pi^L||_m^2. \tag{5.33}$$

By substituting (5.33) into (5.11) and combining the result with (5.28) we have

$$||\pi^L||_m^2 \leq K\Big\{h_p^4 + h_{\hat{c}}^2 + \big(M^*h_{\hat{c}}\big)^2 + (\Delta t)^2\Big\}. \tag{5.34}$$

A similar discussion is adopted for (3.4). Subtracting (5.3a), (5.3b) and (5.3c) at $t=t^{n+1}$ from (3.7a), (3.7b) and (3.7c), respectively, and taking $v=\zeta_T^{n+1}$, $\mathbf{w}=\alpha_T^{n+1}$ and $\mathbf{w}=\bar{\alpha}_T^{n+1}$,

$$\begin{aligned}
&\Big(d_2\frac{T_h^{n+1}-T_h^n}{\Delta t},\zeta_T^{n+1}\Big)_m + \Big(d_{1,T}(P^n,T_h^n)\frac{P^{n+1}-P^n}{\Delta t},\zeta_T^{n+1}\Big)_m + \big(\nabla\cdot\mathbf{G}_T^{n+1},\zeta_T^{n+1}\big)\\
&\quad+\Big(\sum_{s=x,y,z} D_s\alpha_T^{s,n+1},\zeta_T^{n+1}\Big)_m\\
&=\Big(Q(\mathbf{U}^n,P^n,T_h^n,\hat{C}^n) - Q(\mathbf{u}^{n+1},p^{n+1},T^{n+1},\hat{c}^{n+1}) + d_2\frac{\partial T^{n+1}}{\partial t}\\
&\quad+d_{1,T}(p^{n+1},T^{n+1})\frac{\partial p^{n+1}}{\partial t} + \nabla\cdot\mathbf{g}_T^{n+1},\zeta_T^{n+1}\Big)_m,
\end{aligned} \tag{5.35a}$$

$$\sum_{s=x,y,z}\big(\bar{\alpha}_T^{s,n+1},\alpha_T^{s,n+1}\big)_s = \Big(\zeta_T^{n+1},\sum_{s=x,y,z} D_s\alpha_T^{s,n+1}\Big)_m, \tag{5.35b}$$

$$\sum_{s=x,y,z}\big(\alpha_T^{s,n+1},\bar{\alpha}_T^{s,n+1}\big)_s = \sum_{s=x,y,z}\big(E_H\bar{\alpha}_T^{s,n+1},\bar{\alpha}_T^{s,n+1}\big)_s. \tag{5.35c}$$

Summing (5.35a) and (5.35b) and subtracting (5.35c), we have

$$\begin{aligned}
&\Big(d_2\frac{\zeta_T^{n+1}-\zeta_T^n}{\Delta t},\zeta_T^{n+1}\Big)_m + \sum_{s=x,y,z}\big(E_H\bar{\alpha}_T^{s,n+1},\bar{\alpha}_T^{s,n+1}\big)_s\\
=&-\big(\nabla\cdot(\mathbf{G}_T^{n+1}-\mathbf{g}_T^{n+1}),\zeta_T^{n+1}\big)_m + \big(Q(\mathbf{U}^n,P^n,T_h^n,\hat{C}^n) - Q(\mathbf{u}^{n+1},p^{n+1},T^{n+1},\zeta_T^{n+1}\big)_m\\
&+\Big(d_2\Big(\frac{\partial T}{\partial t}-\frac{T^{n+1}-T^n}{\Delta t}\Big),\zeta_T^{n+1}\Big)_m + \Big(d_{1,T}(p^{n+1},T^{n+1})\frac{\partial p^{n+1}}{\partial t}\\
&-d_{1,T}(P^n,T_h^n)\frac{P^{n+1}-P^n}{\Delta t},\zeta_T^{n+1}\Big)_m - \Big(d_2\frac{\zeta_T^{n+1}-\zeta_T^n}{\Delta t},\zeta_T^{n+1}\Big)_m\\
=&\hat{T}_1+\hat{T}_2+\hat{T}_3+\hat{T}_4+\hat{T}_5.
\end{aligned} \tag{5.36}$$

The left-hand side (l.h.s.) of (5.36) is estimated by

$$\text{l.h.s} \geq \frac{1}{2\Delta t}\Big\{\big(d_2\zeta_T^{n+1},\zeta_T^{n+1}\big)_m - \big(d_2\zeta_T^n,\zeta_T^n\big)_m\Big\} + \bar{E}_*|||\bar{\alpha}_T^{n+1}|||^2. \tag{5.37}$$

The terms on the right-hand side are estimated by

$$|\hat{T}_1| = \Big|\big(\nabla\cdot(\mathbf{G}_T^{n+1}-\mathbf{g}_T^{n+1}),\xi_T^{n+1}\big)_m\Big| \le \varepsilon|||\bar{\alpha}_T^{n+1}|||^2 + K\Big\{||\xi_T^{n+1}||_m^2 + h_{\hat{c}}^2\Big\}, \tag{5.38a}$$

$$|\hat{T}_2| \le K\Big\{||\xi_T^{n+1}||_m^2 + ||\xi_T^n||_m^2 + h_p^4 + h_{\hat{c}}^4 + (\Delta t)^2\Big\}, \tag{5.38b}$$

$$|\hat{T}_3| \le K\Big\{\Delta t||\frac{\partial^2 T}{\partial t^2}||^2_{L^2(t^n,t^{n+1};m)} + ||\xi_T^{n+1}||_m^2\Big\}, \tag{5.38c}$$

$$|\hat{T}_4| \le \varepsilon||\partial_t\pi^n||_m^2 + K\Big\{||\xi_T^{n+1}||_m^2 + ||\xi_T^{n+1}||_m^2 + h_p^4 + h_{\hat{c}}^4 + (\Delta t)^2\Big\}. \tag{5.38d}$$

Substituting (5.37) and (5.38) into (5.36), we obtain

$$\begin{aligned}
&\frac{1}{2\Delta t}\Big\{||d_2^{1/2}\xi_T^{n+1}||^2 - ||d_2^{1/2}\xi_T^n||^2\Big\} + \frac{\bar{E}_*}{2}|||\bar{\alpha}_T^{n+1}|||^2 \\
\le& K\Delta t\Big\{||\frac{\partial^2 T}{\partial t^2}||^2_{L^2(t^n,t^{n+1};m)} + ||\frac{\partial^2 p}{\partial t^2}||^2_{L^2(t^n,t^{n+1};m)}\Big\} \\
&+K\Big\{||\xi_T^{n+1}||_m^2 + ||\xi_T^{n+1}||_m^2 + h_p^4 + h_{\hat{c}}^2 + (\Delta t)^2\Big\} + \varepsilon||\partial_t\pi^n||_m^2 \\
&-\Big(d_2\frac{\zeta_T^{n+1}-\zeta_T^n}{\Delta t},\xi_T^{n+1}\Big)_m.
\end{aligned} \tag{5.39}$$

Multiply both sides of (5.39) by $2\Delta t$ and sum them on n ($0\le n\le L-1$). Estimating the last term $-\sum_{n=0}^{L-1}\Big(d_2\frac{\zeta_T^{n+1}-\zeta_T^n}{\Delta t},\xi_T^{n+1}\Big)_m\Delta t$ in a similar discussion of T_5 of (5.14), using $\xi_T^0=0$, (5.28) and the discrete Gronwall's Lemma, we have

$$||\xi_T^L||_m^2 + \sum_{n=0}^{L}|||\bar{\alpha}_T^n|||^2\Delta t \le K\Big\{h_p^4 + h_{\hat{c}}^2 + \big(M^*h_{\hat{c}}\big)^2 + (\Delta t)^2\Big\}. \tag{5.40}$$

Error estimates of the upwind fractional step difference scheme of (1.4) are argued. Let $\xi_{l,ijk}^n = c_l(X_{ijk},t^n) - C_{l,ijk}^n$. Eliminating $C_l^{n+1/3}$, $C_l^{n+2/3}$ and writing a combination equation of (3.8a), (3.8b) and (3.8c) as follow,

$$\begin{aligned}
&\phi_{l,ijk}\frac{C_{l,ijk}^{n+1}-C_{l,ijk}^n}{\Delta t} - \sum_{s=x,y,z}\delta_{\bar{s}}(E_c\delta_s C_l^{n+1})_{ijk} \\
=& -d_1(C_{l,ijk}^n)\frac{P_{ijk}^{n+1}-P_{ijk}^n}{\Delta t} + f_l(\hat{C}_{ijk}^{n+1},C_{1,ijk}^n,C_{2,ijk}^n,\cdots,C_{N,ijk}^n) \\
&-(\Delta t)^2\Big\{\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\partial_t C_l^n))))_{ijk} \\
&+\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t C_l^n))))_{ijk} + \delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t C_l^n))))_{ijk}\Big\} \\
&+(\Delta t)^3\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t C_l^n))))))_{ijk} \\
&-\sum_{s=x,y,z}\delta_{U_s^{n+1}}C_{l,ijk}^n, \quad X_{ijk}\in\Omega_h, \quad l=1,2,\cdots,N.
\end{aligned} \tag{5.41}$$

Making the difference of (1.4) at $(t=t^{n+1})$ and (5.41), we get the error equation of radionuclide factor

$$\begin{aligned}
&\phi_{l,ijk}\frac{\xi_{l,ijk}^{n+1}-\xi_{l,ijk}^{n}}{\Delta t}-\sum_{s=x,y,z}\delta_{\bar{s}}(E_c\delta_s\xi_l^{n+1})_{ijk}\\
=&f_l(\hat{c}_{ijk}^{n+1},c_{1,ijk}^{n+1},c_{2,ijk}^{n+1},\cdots,c_{N,ijk}^{n+1})-f_l(\hat{C}_{ijk}^{n+1},C_{1,ijk}^{n},C_{2,ijk}^{n},\cdots,C_{N,ijk}^{n})\\
&-d_1(C_{l,ijk}^n)\frac{\pi_{ijk}^{n+1}-\pi_{ijk}^{n}}{\Delta t}-\big[d_1(c_{l,ijk}^{n+1})-d_1(C_{l,ijk}^n)\big]\frac{p_{ijk}^{n+1}-p_{ijk}^{n}}{\Delta t}\\
&-(\Delta t)^2\Big\{\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\partial_t\xi_l^n))))_{ijk}+\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n))))_{ijk}\\
&+\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n))))_{ijk}\Big\}+(\Delta t)^3\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n))))))_{ijk}\\
&+\sum_{s=x,y,z}\big[\delta_{U_s^{n+1}}C_{l,ijk}^n-\delta_{u_s^{n+1}}c_{l,ijk}^n\big]+\varepsilon_{l,ijk}^{n+1},\quad X_{ijk}\in\Omega_h,\quad l=1,2,\cdots,N,
\end{aligned}\tag{5.42}$$

where $\big|\varepsilon_{l,ijk}^{n+1}\big|\le K\{h_c^2+\Delta t\}$.

From (5.42),

$$\begin{aligned}
&\phi_{l,ijk}\frac{\xi_{l,ijk}^{n+1}-\xi_{l,ijk}^{n}}{\Delta t}-\sum_{s=x,y,z}\delta_{\bar{s}}(E_c\delta_s\xi_l^{n+1})_{ijk}\\
\le&K\Big\{\sum_{l=1}^{N}\big|\xi_{l,ijk}^n\big|+\big|\xi_{\hat{c},ijk}^{n+1}\big|+\big|\mathbf{u}_{ijk}^{n+1}-\mathbf{U}_{ijk}^n\big|+h_p^2+h_{\hat{c}}^2+\Delta t\Big\}-d_1(C_{l,ijk}^n)\frac{\pi_{ijk}^{n+1}-\pi_{ijk}^{n}}{\Delta t}\\
&-(\Delta t)^2\Big\{\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\partial_t\xi_l^n))))_{ijk}+\cdots+\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n))))_{ijk}\Big\}\\
&+(\Delta t)^3\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n))))))_{ijk}\\
&+\sum_{s=x,y,z}\big[\delta_{U_s^{n+1}}C_{l,ijk}^n-\delta_{u_s^{n+1}}c_{l,ijk}^n\big],\quad X_{ijk}\in\Omega_h.
\end{aligned}\tag{5.43}$$

Multiplying both sides of (5.43) by $\partial_t\xi_{l,ijk}^n\Delta t=\xi_{l,ijk}^{n+1}-\xi_{l,ijk}^n$ and using the summation by parts, we have an inner product formulation,

$$\begin{aligned}
&\Big\langle\phi_l\frac{\xi_l^{n+1}-\xi_l^n}{\Delta t},\partial_t\xi_l^n\Big\rangle\Delta t+\frac{1}{2}\sum_{s=x,y,z}\Big\{\big\langle E_c\delta_s\xi_l^{n+1}),\delta_s\xi_l^{n+1}\big\rangle-\big\langle E_c\delta_s\xi_l^{n}),\delta_s\xi_l^{n}\big\rangle\Big\}\\
\le&\varepsilon\big|\partial_t\xi_l^n\big|_0^2\Delta t+K\Big\{\sum_{l=1}^{N}\big|\xi_l^n\big|_0^2+\big|\xi_{\hat{c}}^{n+1}\big|_0^2+\big|\big|\big|\sigma^{n+1}\big|\big|\big|^2+h_p^4+h_{\hat{c}}^2+h_c^4+(\Delta t)^2\Big\}\Delta t\\
&-\big\langle d_1(C_l^n)\partial_t\pi^n,\partial_t\zeta_l^n\big\rangle\Delta t-(\Delta t)^3\Big\{\big\langle\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\partial_t\xi_l^n)))),\partial_t\xi_l^n\big\rangle\\
&+\cdots+\big\langle\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}\cdot(E_c\delta_z(\partial_t\xi_l^n)))),\partial_t\xi_l^n\big\rangle\Big\}
\end{aligned}\tag{5.44}$$

$$
\begin{aligned}
&+(\Delta t)^4\Big\langle \delta_{\bar{x}}\big(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n))))))\big),\partial_t\xi_l^n\Big\rangle \\
&+\Big\langle \sum_{s=x,y,z}\big[\delta_{U_s^{n+1}}C_l^n-\delta_{u_s^{n+1}}c_l^n\big],\partial_t\xi_l^n\Big\rangle\Delta t,
\end{aligned} \tag{5.45}
$$

where $\langle\cdot,\cdot\rangle$ and $|\cdot|_0$ denote the discrete inner product and discrete norm in l^2 space, respectively. The relation of continuous $L^2(\Omega)$-norm and discrete $l^2(\Omega)$-norm is used [39]. Rewrite (5.44) in the following formulation

$$
\begin{aligned}
&\Big\langle \phi_l\frac{\xi_l^{n+1}-\xi_l^n}{\Delta t},\partial_t\xi_l^n\Big\rangle\Delta t+\frac{1}{2}\sum_{s=x,y,z}\Big\{\big\langle E_c\delta_s\xi_l^{n+1}),\delta_s\xi_l^{n+1}\big\rangle-\big\langle E_c\delta_s\xi_l^n),\delta_s\xi_l^n\big\rangle\Big\} \\
\le& K\Big\{\sum_{l=1}^{N}\big|\xi_l^n\big|_0^2+\big|\xi_{\hat{c}}^{n+1}\big|_0^2+\big|\big|\big|\sigma^{n+1}\big|\big|\big|^2+\big|\partial_t\pi^n\big|_0^2+h_p^4+h_{\hat{c}}^2+h_c^4+(\Delta t)^2\Big\}\Delta t \\
&-(\Delta t)^3\Big\{\big\langle\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\partial_t\xi_l^n)))),\partial_t\xi_l^n\big\rangle+\cdots+\big\langle\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n)))),\partial_t\xi_l^n\big\rangle\Big\} \\
&+(\Delta t)^4\big\langle\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n)))))),\partial_t\xi_l^n\big\rangle+\varepsilon\big|\partial_t\xi_l^n\big|_0^2\Delta t \\
&+\Big\langle\sum_{s=x,y,z}\big[\delta_{U_s^{n+1}}C_l^n-\delta_{u_s^{n+1}}c_l^n\big],\partial_t\xi_l^n\Big\rangle\Delta t.
\end{aligned} \tag{5.46}
$$

The second part on the right-hand side of (5.46) is estimated. Consider the first term

$$
\begin{aligned}
&-(\Delta t)^3\big\langle\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\partial_t\xi_l^n)))),\partial_t\xi_l^n\big\rangle \\
=&-(\Delta t)^3\Big\{\big\langle\delta_x(E_c\delta_y(\partial_t\xi_l^n)),\delta_y(\phi_l^{-1}E_c\delta_x(\partial_t\xi_l^n))\big\rangle+\big\langle E_c\delta_y(\partial_t\xi_l^n),\delta_y(\delta_x\phi_l^{-1}\cdot E_c\delta_x(\partial_t\xi_l^n))\big\rangle\Big\} \\
=&-(\Delta t)^3\sum_{\Omega_h}\Big\{E_{c,i,j+1/2,k}E_{c,i+1/2,jk}\phi_{l,ijk}^{-1}(\delta_x\delta_y\delta_t\xi_l^n)_{ijk}^2+\big[E_{c,i,j+1/2,k}\delta_y(E_{c,i+1/2,jk}\phi_{l,ijk}^{-1})\cdot\delta_x(\partial_t\xi_{l,ijk}^n) \\
&+E_{c,i+1/2,jk}\phi_{l,ijk}^{-1}\delta_xE_{c,i,j+1/2,k}\cdot\delta_y(\partial_t\xi_{l,ijk}^n)+E_{c,i,j+1/2,k}E_{c,i+1/2,jk}\delta_y(\partial_t\xi_{l,ijk}^n)\big]\cdot\delta_x\delta_y(\partial_t\xi_{l,ijk}^n) \\
&+\big[E_{c,i,j+1/2,k}E_{c,i+1/2,jk}\delta_x\delta_y\phi_{l,ijk}^{-1} \\
&+E_{c,i,j+1/2,k}\delta_yE_{c,i+1/2,jk}\delta_x\delta_y\phi_{l,ijk}^{-1}\big]\delta_x(\partial_t\xi_{l,ijk}^n)\cdot\delta_y(\partial_t\xi_{l,ijk}^n)\Big\}h_i^xh_j^yh_k^z.
\end{aligned} \tag{5.47}
$$

Using the positive definiteness of E_c and eliminating high-order difference quotient $\delta_x\delta_y(\partial_t\xi_l^n)$ by Cauchy inequality, we get

$$
\begin{aligned}
&-(\Delta t)^3\sum_{\Omega_h}\Big\{E_{c,i,j+1/2,k}E_{c,i+1/2,jk}\phi_{l,ijk}^{-1}(\delta_x\delta_y\delta_t\xi_{l,ijk})^2+\cdots\Big\}h_i^xh_j^yh_k^z \\
\le& K\Big\{\big|\nabla_h\xi_l^{n+1}\big|_0^2+\big|\nabla_h\xi_l^n\big|_0^2\Big\}\Delta t,
\end{aligned} \tag{5.48}
$$

where $|\nabla_h\xi_l|_0^2=\sum_{s=x,y,z}|\delta_s\xi_l|_0^2$.

Similarly, we complete the estimates of the second and third parts of (5.46). Thus,

$$\begin{aligned}
&-(\Delta t)^3\Big\{\big\langle\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\partial_t\xi_l^n)))),\partial_t\xi_l^n\big\rangle+\cdots\\
&\quad+\big\langle\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n)))),\partial_t\xi_l^n\big\rangle\Big\}\\
&\quad+(\Delta t)^4\big\langle\delta_{\bar{x}}(E_c\delta_x(\phi_l^{-1}\delta_{\bar{y}}(E_c\delta_y(\phi_l^{-1}\delta_{\bar{z}}(E_c\delta_z(\partial_t\xi_l^n)))))),\partial_t\xi_l^n\big\rangle\\
\le& K\Big\{\big|\nabla_h\xi_l^{n+1}\big|_0^2+\big|\nabla_h\xi_l^n\big|_0^2\Big\}\Delta t. \qquad (5.49)
\end{aligned}$$

The fourth part is estimated by

$$\begin{aligned}
&\Big\langle\sum_{s=x,y,z}\big[\delta_{U_s^{n+1}}C_l^n-\delta_{u_s^{n+1}}c_l^n\big],\partial_t\xi_l^n\Big\rangle\Delta t\\
\le&\varepsilon\big|\big|\partial_t\xi_l^n\big|\big|^2\Delta t+K\Big\{\big|\big|\big|\sigma^n\big|\big|\big|^2+\big|\nabla_h\xi_l^n\big|_0^2+h_p^4+(\Delta t)^2\Big\}. \qquad (5.50)
\end{aligned}$$

Applying (5.48)-(5.50),

$$\begin{aligned}
&\big|\partial_t\xi_l^n\big|_0^2\Delta t+\frac{1}{2}\sum_{s=x,y,z}\Big\{\big\langle E_c\delta_s\xi_l^{n+1}),\delta_s\xi_l^{n+1}\big\rangle-\big\langle E_c\delta_s\xi_l^n),\delta_s\xi_l^n\big\rangle\Big\}\\
\le& K\Big\{\sum_{l=1}^N\big[\big|\xi_l^n\big|_0^2+\big|\nabla_h\xi_l^{n+1}\big|_0^2+\big|\nabla_h\xi_l^n\big|_0^2\big]+\big|\xi_{\hat{c}}^{n+1}\big|_0^2+\big|\big|\big|\sigma^{n+1}\big|\big|\big|^2+\big|\partial_t\pi^n\big|_0^2+h_p^4+h_{\hat{c}}^2\\
&+h_c^4+(\Delta t)^2\Big\}\Delta t+\varepsilon\big|\partial_t\xi_l^n\big|_0^2\Delta t. \qquad (5.51)
\end{aligned}$$

Summing (5.51) on l $(1\le l\le N)$ then on t $(0\le n\le L)$, noting that $\xi_l^0=0, l=1,2,\cdots,N$ and using (5.28) and (5.34), we obtain

$$\begin{aligned}
&\sum_{n=0}^L\sum_{l=1}^N\big|\partial_t\xi_l^n\big|_0^2\Delta t+\frac{1}{2}\sum_{l=1}^N\sum_{s=x,y,z}\big\langle E_c\delta_s\xi_l^{L+1},\delta_s\xi_l^{L+1}\big\rangle\\
\le& K\sum_{n=0}^L\big|\partial_t\pi^n\big|_0^2\Delta t+K\Big\{\sum_{n=0}^L\sum_{l=1}^N\big[\big|\xi_l^n\big|_0^2+\big|\nabla_h\xi_l^{n+1}\big|_0^2\big]+h_p^4+h_{\hat{c}}^2\\
&+(M^*h_{\hat{c}})^2+h_c^4+(\Delta t)^2\Big\}\Delta t. \qquad (5.52)
\end{aligned}$$

Here $\big|\xi_l^{L+1}\big|_0^2\le\varepsilon\sum_{n=0}^L\big|\partial_t\xi_l^n\big|_0^2\Delta t+K\sum_{n=0}^L\big|\xi_l^n\big|_0^2\Delta t$ is used. Using the relation of $L^2(\Omega)$-norm and l^2-norm [8,39], (5.28), (5.34) and the Gronwall's lemma, we have

$$\sum_{n=0}^L\sum_{l=1}^N\big|\partial_t\xi_l^n\big|_0^2\Delta t+\sum_{l=1}^N\big[\big|\xi_l^n\big|_0^2+\big|\nabla_h\xi_l^{n+1}\big|_0^2\big]\le K\Big\{h_p^4+h_{\hat{c}}^2+(M^*h_{\hat{c}})^2+h_c^4+(\Delta t)^2\Big\}. \qquad (5.53)$$

The following theorem is concluded from (5.28), (5.34), (5.40), (5.53) and Lemma 5.1.

Theorem 5.1. *Suppose that the problem of* (1.1)-(1.6) *satisfies (R) and (C). Adopt the composite scheme of* (3.5), (3.6), (3.7) *and* (3.8) *to obtain numerical solutions. Then,*

$$\begin{aligned}&||p-P||_{\bar{L}^\infty(J;m)}+||\partial_t(p-P)||_{\bar{L}^2(J;m)}+||\mathbf{u}-\mathbf{U}||_{\bar{L}^\infty(J;V)}+||\hat{c}-\hat{C}||_{\bar{L}^\infty(J;m)}+||\bar{\mathbf{z}}-\bar{\mathbf{Z}}||_{\bar{L}^2(J;V)}\\&\quad+||T-T_h||_{\bar{L}^\infty(J;m)}+||\bar{\mathbf{z}}_T-\bar{\mathbf{Z}}_T||_{\bar{L}^2(J;V)}+\sum_{l=1}^{N}\Big\{||c_l-C_l||_{\bar{L}^\infty(J;h^1)}+||\partial_t(c_l-C_l)||_{\bar{L}^2(J;l^2)}\Big\}\\&\leq M^{**}\Big\{h_p^2+h_{\hat{c}}+M^*h_{\hat{c}}+h_c^2+\Delta t\Big\},\end{aligned}\tag{5.54}$$

where

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

and the constant M^{**} depends on p, $\hat{c}$, c_l $(l=1,2,\cdots,N)$, T and their derivatives.

Next, an improved composite scheme on a changing mesh of (3.5)-(3.8) is discussed. (3.5) and (3.8) are not changed for the pressure and the concentration of radionuclide. (3.6) and (3.7) are improved by a linear approximation for the concentration of brine and temperature. The linear approximation to $\hat{C}^{n-1}$ is used to replace L^2-projection, and an optimal error estimates is concluded on a changing mesh.

Consider the improvement for (3.6). Given $\hat{C}^n\in S_h^n$, a linear function is defined on e^n by $\bar{\hat{C}}^n$,

$$\bar{\hat{C}}^n\big|_{e^n}=\hat{C}^n(x_e^n)+(x-x_e^n)\cdot\delta\hat{C}_e^n,\tag{5.55}$$

where x_e^n is the barycenter of e^n and $\delta\hat{C}_e^n$ is the gradient or the slope of numerical function obtained by the mixed volume element, $-\bar{\mathbf{Z}}^n$,

$$\delta\hat{C}_e^n=-\frac{1}{\mathrm{mes}(e^n)}\int_{e^n}\bar{\mathbf{Z}}^n(x)dx.\tag{5.56}$$

The procedures of (3.6b) and (3.6c) are not changed, and (3.6a) is replaced by

$$\begin{aligned}&\Big(\phi(x)\frac{\hat{C}^{n+1}-\bar{\hat{C}}^n}{\Delta t},v\Big)_m+\Big(\phi\hat{C}^n\frac{P^{n+1}-P^n}{\Delta t},v\Big)_m+\big(\nabla\cdot\mathbf{G}^{n+1},v\big)_m+\Big(\sum_{s=x,y,z}D_sZ^{s,n+1},v\Big)_m\\&=\big(F(\hat{C}^n),v\big)_m,\quad \forall v\in S_h^{n+1}.\end{aligned}\tag{5.57}$$

The computation of $\bar{\hat{C}}^n$ is added only if the mesh changes. If the mesh is unchanged, $S_h^n=S_h^{n+1}$, then

$$\big(\phi\bar{\hat{C}}^n,v\big)_m=\big(\phi\hat{C}^n,v\big)_m.\tag{5.58}$$

We use a similar discussion to give the estimates. (5.12b) and (5.12c) are still true. (5.12a) is changed into

$$\begin{aligned}
&\Big(\phi\frac{\xi_{\hat{c}}^{n+1}-\xi_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m+\Big(\sum_{s=x,y,z}E_c\bar{\alpha}_{\hat{c}}^{s,n+1},\bar{\alpha}_{\hat{c}}^{s,n+1}\Big)_m\\
=&-\big(\nabla\cdot(\mathbf{G}^{n+1}-\mathbf{g}^{n+1}),\xi_{\hat{c}}^{n+1}\big)_m+\big(F(\hat{C}^n)-F(\hat{c}^{n+1}),\xi_{\hat{c}}^{n+1}\big)_m\\
&+\Big(\phi\hat{c}^{n+1}\frac{\partial p^{n+1}}{\partial t}-\phi\hat{C}^n\frac{P^{n+1}-P^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m+\Big(\phi\frac{\partial\hat{c}^{n+1}}{\partial t}-\phi\frac{\hat{c}^{n+1}-\hat{c}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\\
&+\Big(\phi\frac{\bar{\xi}_{\hat{c}}^{n+1}-\xi_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m-\Big(\phi\frac{\hat{c}^n-\bar{\Pi}\hat{c}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m,
\end{aligned}\tag{5.59}$$

where $\bar{\xi}_{\hat{c}}^n=\bar{\hat{C}}^n-\bar{\Pi}\hat{c}^n$. $\bar{\Pi}\hat{c}^n$ is defined by

$$\bar{\Pi}\hat{c}^n\big|_{e^n}=\Pi\hat{c}^n(x_e^n)-(x-x_e^n)\cdot\Big(\frac{1}{\text{mes}(e^n)}\int_{e^n}\Pi\bar{\mathbf{z}}^n(x)dx\Big),\tag{5.60}$$

where Π is the projection operator in (5.2), that is, $\Pi\hat{c}^n=\tilde{\hat{c}}^n$, $\Pi\bar{\mathbf{z}}^n=\tilde{\bar{\mathbf{z}}}^n$.

The first four terms of (5.59) have the same estimates as above. The other terms are addressed now. It holds obviously

$$\Big(\phi\frac{\bar{\xi}_{\hat{c}}^{n}-\xi_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n}\Big)_m\le\frac{\phi^*}{\Delta t}||\bar{\xi}_{\hat{c}}^n-\xi_{\hat{c}}^n||_m\cdot||\xi_{\hat{c}}^{n+1}||_m\le\frac{\varepsilon}{(\Delta t)^2}||\bar{\xi}_{\hat{c}}^n-\xi_{\hat{c}}^n||_m^2+K||\xi_{\hat{c}}^{n+1}||_m^2.\tag{5.61}$$

From (5.55), (5.56) and (5.60), we have

$$||\bar{\xi}_{\hat{c}}^n-\xi_{\hat{c}}^n||^2=\sum_i\int_{e_i}|\bar{\xi}_{\hat{c}}^n-\xi_{\hat{c}}^n|^2dx=\sum_i\int_{e_i}\Big|(x-x_e^n)\frac{1}{\text{mes}(e^n)}\int_{e_i}\bar{\alpha}_{\hat{c}}^n dy\Big|^2dx.\tag{5.62}$$

Substituting (5.62) into (5.61) and assuming that it holds $h_{\hat{c}}=\mathcal{O}(\Delta t)$, we have

$$\Big(\phi\frac{\bar{\xi}_{\hat{c}}^{n}-\xi_{\hat{c}}^{n}}{\Delta t},\xi_{\hat{c}}^{n}\Big)_m\le\frac{\varepsilon(h_{\hat{c}})^2}{(\Delta t)^2}|||\bar{\alpha}_{\hat{c}}^n|||^2+K||\xi_{\hat{c}}^{n+1}||_m^2\le\varepsilon|||\bar{\alpha}_{\hat{c}}^n|||^2+K||\xi_{\hat{c}}^{n+1}||_m^2.\tag{5.63}$$

The last term of (5.59) is considered. We note that

$$-\Big(\phi\frac{\hat{c}^n-\bar{\Pi}\hat{c}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\le\frac{\varepsilon}{(\Delta t)^2}||\hat{c}^n-\bar{\Pi}\hat{c}^n||_m^2+K||\xi_{\hat{c}}^{n+1}||_m^2.\tag{5.64}$$

Using the Taylor expansion, for $\forall x\in e^n$, we have

$$\begin{aligned}
\hat{c}^n(x)&=\hat{c}^n(x_e^n)-(x-x_e^n)\cdot\bar{\mathbf{z}}^n(x_e^n)+\mathcal{O}((h_{\hat{c}})^2)\\
&=\Pi\hat{c}^n(x_e^n)-(x-x_e^n)\frac{1}{\text{mes}(e^n)}\int_{e^n}\bar{\mathbf{z}}^n dy+\mathcal{O}((h_{\hat{c}})^2),
\end{aligned}\tag{5.65}$$

where

$$\hat{c}^n(x_e^n)-\Pi\hat{c}^n(x_e^n)=\mathcal{O}((h_{\hat{c}})^2) \quad \text{and} \quad \Big|\bar{\mathbf{z}}^n(x_e^n)-\frac{1}{\text{mes}(e^n)}\int_{e^n}\bar{\mathbf{z}}^n dy\Big|=\mathcal{O}((h_{\hat{c}})^2)$$

are used. Thus,

$$\begin{aligned}||\hat{c}^n-\bar{\Pi}\hat{c}^n||_m^2=&\sum_i\int_{e_i}\Big|(x-x_e^n)\frac{1}{\text{mes}(e^n)}\int_{e^n}\bar{\beta}_{\hat{c}}^n dy+\mathcal{O}((h_{\hat{c}})^2)\Big|^2dx\\ \le&K(h_{\hat{c}})^2|||\bar{\beta}_{\hat{c}}^n|||^2+K(h_{\hat{c}})^4\le K(h_{\hat{c}})^4.\end{aligned} \tag{5.66}$$

Substituting (5.66) into (5.64),

$$-\Big(\phi\frac{\hat{c}^n-\bar{\Pi}\hat{c}^n}{\Delta t},\xi_{\hat{c}}^{n+1}\Big)_m\le K(h_{\hat{c}})^2+K||\xi_{\hat{c}}^{n+1}||_m^2. \tag{5.67}$$

Substituting (5.63) and (5.67) into (5.59), multiplying both sides of the resulting equation by $2\Delta t$, summing them on $n=1,2,\cdots,L-1$ and using $\xi_{\hat{c}}^0=0$ and the discrete Gronwall's lemma, we have

$$||\phi^{1/2}\xi_{\hat{c}}^L||_m^2+\sum_{n=0}^{L}|||\bar{\alpha}_{\hat{c}}^n|||^2\Delta t\le K\{h_{\hat{c}}^2+(\Delta t)^2\}. \tag{5.68}$$

(3.7) is estimated similarly. Then,

$$||d_2^{1/2}\xi_T^L||_m^2+\sum_{n=0}^{L}|||\bar{\alpha}_T^n|||^2\Delta t\le K\{h_{\hat{c}}^2+(\Delta t)^2\}. \tag{5.69}$$

Combining (5.26), (5.34), (5.68), (5.69), (5.54) and Lemma 5.1, we have the following theorem.

Theorem 5.2. *Suppose that the problem of* (1.1)-(1.6) *is regular (R) and positive definite (C). Adopt the modified scheme on a changing mesh to obtain numerical solutions. If the partition satisfies $h_{\hat{c}}=\mathcal{O}(\Delta t)$, then we have the following optimal order error estimates*

$$\begin{aligned}&||p-P||_{\bar{L}^\infty(J;m)}+||\partial_t(p-P)||_{\bar{L}^2(J;m)}+||\mathbf{u}-\mathbf{U}||_{\bar{L}^\infty(J;V)}\\ &\le M^{***}\{h_p^2+h_{\hat{c}}+\Delta t\},\end{aligned} \tag{5.70a}$$

$$\begin{aligned}&||\hat{c}-\hat{C}||_{\bar{L}^\infty(J;m)}+||\bar{\mathbf{z}}-\bar{\mathbf{Z}}||_{\bar{L}^2(J;V)}+||T-T_h||_{\bar{L}^\infty(J;m)}+||\bar{\mathbf{z}}_T-\bar{\mathbf{Z}}_T||_{\bar{L}^2(J;V)}\\ &\quad+\sum_{l=1}^{N}\Big\{||c_l-C_l||_{\bar{L}^\infty(J;h^1)}+||\partial_t(c_l-C_l)||_{\bar{L}^2(J;l^2)}\Big\}\\ &\le M^{***}\Big\{h_p^2+h_{\hat{c}}+h_c^2+\Delta t\Big\},\end{aligned} \tag{5.70b}$$

where M^{***} is a positive constant dependent on p, $\hat{c}$, c_l $(l=1,2,\cdots,N)$, T and their derivatives.

6 Numerical example

In this section, a simplified displacement problem is solved by the present scheme. Suppose that the pressure and the Darcy velocity are known. Consider the concentration equation

$$\frac{\partial c}{\partial t}+c_x-ac_{xx}=f, \tag{6.1}$$

where $t\in(0,\frac{1}{2})$, $x\in[0,\pi]$, $a=1.0\times 10^{-4}$, that is to say that (6.1) is convection dominated. Exact solution is defined by $c=\exp(-0.05t)(\sin(x-t))^{20}$, and f is obtained naturally. Exact solution has a sharp front in the interval $[1.5,2.5]$ as shown in Fig. 2, which moves with respect to t. Since finite element method gives rise to numerical oscillation, so we adopt upwind-mixed volume element method on changing meshes. Here we change the partition once, and get satisfactory numerical results without numerical oscillation or dispersion (see Fig. 3. The oscillation figure obtained by finite element method is illustrated in Fig. 4.

From Figs. 2-4, we conclude that the upwind-mixed finite element approximates convection-dominate diffusion problems well in comparison with finite element method. Error estimates in L^2-norm at different positions are compared in Table 1. STATIC denotes the upwind-mixed volume element on a statistic partition, and MOVE denotes the scheme on changing meshes. The method on changing meshes can solve convection-dominated diffusion problems well and has on order of accuracy consistent with the theoretical result.

Remark 6.1. In actual computations, numerical data are bad when time step is independent of space step. The approximations are accurate when time step is almost equal to space step. The numerical conclusion is consistent with Theorem 5.1.

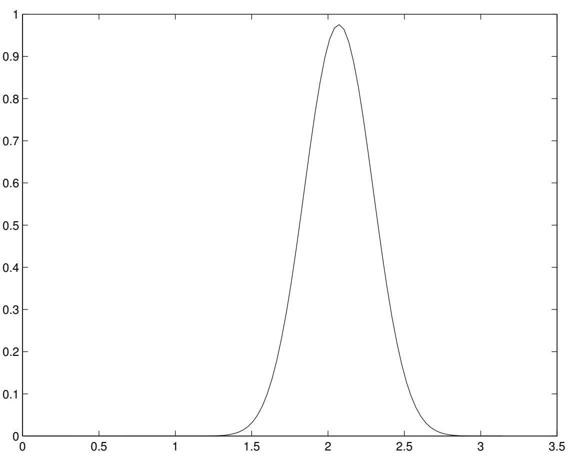

Figure 2: Exact solution at $t=\frac{1}{2}$.

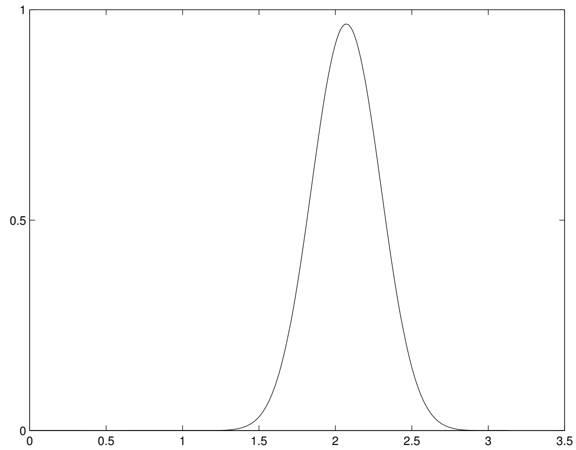

Figure 3: Numerical solution on changing meshes.

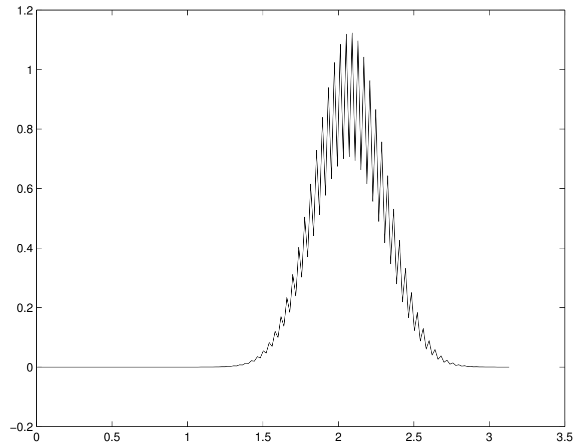

Figure 4: Oscillated illustration of finite element method.

Table 1: Error estimates at $t=1/2$.

h	$\pi/60$	$\pi/80$	$\pi/100$	$\pi/120$
STATIC	$7.70e-003$	$3.89e-003$	$2.11e-003$	$1.23e-003$
MOVE	$1.59e-003$	$5.5064e-004$	$1.6198e-004$	$2.8174e-005$

7 Conclusions and discussions

An upwind mixed volume element-fractional step difference scheme is proposed and its convergence analysis is shown for the disposal of compressible nuclear waste contamination. In Section 1, mathematical model, physical background and related research are introduced. In Section 2, the partitions, notations and preliminary statements are prepared for constructing the procedures and convergence analysis. In Section 3, the composite procedures including mixed volume element, upwind approximation and fractional step difference are constructed. The flow equation is approximated by a conservative mixed volume element scheme. The computational accuracy of Darcy velocity is improved by one order. The conservative upwind mixed volume element is used to solve the concentration equation of brine and the heat conduction equation, where the diffusion and convection are treated by mixed volume element and upwind difference, respectively. The upwind method can solve convection-dominated diffusion equations well because it avoids numerical dispersion and nonphysical oscillation and confirms high accuracy. The mixed volume element can compute the concentration and temperature and their adjoint vector functions simultaneously. It has the nature of elemental conservation of mass or energy which is important in numerical simulation of underground seepage mechanics. The concentrations of radionuclide factors are computed by the method of upwind fractional step difference in parallel, where the whole computation is divided into three one-dimensional problem and the simple speedup solver is used. So the computational workload is decreased greatly. In Section 4, The elemental conservation of mass or energy is proved. In Section 5, we apply the theory and technique of a priori estimates to show optimal order error estimates. In Section 6, numerical examples of a simplified model are discussed to illustrate theoretical analysis and show the feasibility of the presented composite scheme. Several interesting conclusions are stated as follows.

(I) The compressibility is involved in the present paper. The scheme has the conservation of mass or energy, an important nature in numerical simulation of seepage mechanics.

(II) The presented scheme combines mixed volume element, upwind approximation and fractional step difference, so it has many merits such as high accuracy, strong stability and the feasibility in solving large-scale actual engineering problems on three-dimensional complicated region.

(III) This discussion improves the research on nuclear waste contamination disposal [1, 2, 12, 33, 34]. The method presented by the research group of Ewing only solves two-dimensional problem and the conservation of mass or energy does not hold.

(IV) This discussion improves the mixed finite element on changing meshes by Dawson and Kirby in [32], where they gave an optimal result only for a simple parabolic and a special changing mesh. Here we obtain an optimal convergence rate for numerical scheme on general changing meshes.

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