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A MIXED VOLUME ELEMENT WITH CHARACTERISTIC MIXED VOLUME ELEMENT FOR CONTAMINATION TRANSPORT PROBLEM

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Abstract

Nonlinear systems of convection-dominated diffusion equations are used as the mathematical model of contamination transport problem which is an important topic in environmental protection science. An elliptic equation defines the pressure, a convection-diffusion equation expresses the concentration of contamination, and an ordinary differential equation interprets the surface absorption concentration. The transport pressure appears in the equation of the concentration which determines the Darcy velocity and also controls the physical process. The method of conservative mixed volume element is used to solve the flow equation which improves the computational accuracy of Darcy velocity by one order. We use the mixed volume element with the characteristic to approximate the concentration. This method of characteristic not only preserves the strong computational stability at sharp front, but also eliminates numerical dispersion and nonphysical oscillation. In the present scheme, we could adopt a large step without losing accuracy. The diffusion is approximated by the mixed volume element. The concentration and its adjoint vector function are obtained simultaneously, and the locally conservative law is preserved. We derive an optimal second order estimates in l^2-norm by using the theory and technique of a priori estimates of a differential equation. From the numerical examples given in the paper, the method shows its potential to be a powerful tool in solving actual problems.

1. Introduction

Numerical simulation of the contamination transport problem is an efficient way to find how to protect the environment and treat the pollution. The physical interpretation is given by a mathematical system of partial differential equations. In this model, an elliptic equation defines the pressure, a convection-diffusion equation expresses the concentration of contamination, and an ODE interprets the surface absorption concentration. We provide a simplified physical background in the following. When the chemical substances are dissolved in the underground water, the substances are absorbed by the surface of the media, and then the chemical reaction takes place. The chemical reaction also affects the transportation of the solutes as the underground water

moves. Consideration of the reaction helps us to understand how the contamination transport in terms of time and space. The reaction speed depends on the absorption. The equilibrium is denoted by quick reaction, and non-equilibrium absorption is denoted by slow reaction speed. In this paper, we discuss the non-equilibrium absorption. The following mathematical model is discussed with the initial-boundary value conditions [12, 13, 18, 31]:

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

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

$$\theta(X)\frac{\partial c}{\partial t} + \rho(X)\frac{\partial s}{\partial t} + \nabla \cdot (\mathbf{u}c) - \nabla \cdot (\theta D \nabla c) = 0,\ X \in \Omega,\ t \in J, \tag{1.2}$$

$$\frac{\partial s}{\partial t} = \hat{\alpha}(\phi(c) - s),\ X \in \Omega,\ t \in J, \tag{1.3}$$

where Ω is a bounded domain in $\mathbb{R}^3$, $p(X, t)$ denotes the pressure, and $\mathbf{u} = (u_x, u_y, u_z)^T$ is Darcy velocity. The functions $c(X, t)$ and $s(X, t)$ denote the contamination concentration and non-equilibrium absorption concentration, $\kappa(c)$ is the permeability, $\theta(X)$ and $\rho(X)$, two positive functions, are water storage rates of moving water and the density, respectively, D is a total matrix of molecular diffusion and chemical dispersion,

$$\begin{aligned}\theta D(X, \mathbf{u}) = {} & \theta D_{\mathrm{mol}}(X)\mathbf{I} + \alpha_l |\mathbf{u}|^{\beta} \begin{pmatrix} \hat{u}_x^2 & \hat{u}_x\hat{u}_y & \hat{u}_x\hat{u}_z \\ \hat{u}_y\hat{u}_x & \hat{u}_y^2 & \hat{u}_y\hat{u}_z \\ \hat{u}_z\hat{u}_x & \hat{u}_z\hat{u}_y & \hat{u}_z^2 \end{pmatrix} \\ & + \alpha_t |\mathbf{u}|^{\beta} \begin{pmatrix} \hat{u}_y^2 + \hat{u}_z^2 & -\hat{u}_x\hat{u}_y & -\hat{u}_x\hat{u}_z \\ -\hat{u}_x\hat{u}_y & \hat{u}_x^2 + \hat{u}_z^2 & -\hat{u}_y\hat{u}_z \\ -\hat{u}_x\hat{u}_z & -\hat{u}_z\hat{u}_y & \hat{u}_x^2 + \hat{u}_y^2 \end{pmatrix}, \end{aligned} \tag{1.4}$$

$D_{\mathrm{mol}}(X)$ is a molecular diffusion matrix and $\mathbf{I}$ is a 3×3 identity matrix; α_l and α_t, respectively represent longitudinal and transverse diffusion coefficients; $\hat{u}_x$, $\hat{u}_y$ and $\hat{u}_z$ are three direction cosines of Darcy velocity $\mathbf{u}$. Generally speaking, β is a constant not less than 2, and diffusion-dispersion matrix is positive definite. Here we only consider the molecular diffusion. Suppose that $D_* \le D_{\mathrm{mol}}(X) \le D^*$ holds for positive constants D_* and D^*. $\hat{\alpha}$, a positive constant, is the exchange coefficient. $\phi(c)$ denotes the isothermal absorption, generally defined by two different methods

(I) Langmuir isotherm, $\phi(c) = \dfrac{k_1 c}{1 + k_2 c}$, $k_1, k_2 > 0$,

(II) Freundlinch isotherm, $\phi(c) = k_3 c^p$, $k_3 > 0$, where $p \in [0, 1]$.

The case (II) is a degraded parabolic equation for $p < 1$, and $\phi \in C^0 \bigcap C^1((-\infty, 0) \bigcup (0, \infty))$ is an increasing function with $\phi(0) = 0$. Since the parameter $p \in (0, 1)$ is locally Hölder continuous, thus the regularity of c decreases. $q(X, t)$ is the source and sink term. Three unknown functions are $p(X, t)$, $c(X, t)$, and $s(X, t)$.

Assume that the mixture is impermeable across the boundary,

$$\mathbf{u} \cdot \nu = 0,\ X \in \partial\Omega,\ (\theta D \nabla c - c\mathbf{u}) \cdot \nu = 0,\ X \in \partial\Omega,\ t \in J, \tag{1.5}$$

where ν denotes the outer normal vector at the boundary $\partial\Omega$ of Ω.

The initial conditions are defined by

$$c(X, 0) = c_0(X),\ s(X, 0) = s_0(X),\ X \in \Omega. \tag{1.6}$$

The following restriction is introduced to confirm the existence and uniqueness:

$$\int_\Omega q(X, t) dX = 0,\ \int_\Omega p(X, t) dX = 0,\ t \in J. \tag{1.7}$$

The Lipschitz continuity does not hold for this physical model, and this nonlinearity decreases the regularity. It brings trouble on numerical analysis for the full discrete scheme. Dawson first presents and analyzes the method of characteristics-Galerkin for non-equilibrium absorption in [12, 13]. While numerical oscillation possibly appears and the local conservation of mass is lost. Furthermore, an upwind with mixed finite element method is put forward to discuss a nonlinear contamination transport equation with equilibrium absorption in one variable. Convergence analysis is shown only for a local low-order semidiscrete algorithm. It is well-known that standard finite element could not solve convection-diffusion problems well because of strong numerical oscillation. In order to treat this problem well, some efficient numerical methods are put forward such as characteristic difference, characteristic finite element [17, 34-36], upstream-weighted finite difference [30], high-order Godunov scheme [3], streamline diffusion method [21], least squares mixed finite element [33], modified method of characteristics with Galerkin finite element (MMOC-Galerkin) [11], Eulerian-Lagrangian localized adjoint method (ELLAM) [6] and so on. These methods improve traditional finite element method while they have some natural faults. Upstream weighted difference method could introduce numerical dispersion into the solution near the sharp fronts. High-order Godunov scheme requires an additional CTL restriction with respect to time step. Streamline diffusion method and least squares mixed finite element method reduce numerical dispersion but add some numerical work to define and handle artificial streamline directions. ELLAM confirms the local conservation of mass but need a large-scale computation to evaluate the resulting integrals. Arbogast and Wheeler [2] present a type of characteristic mixed finite element to solve the convection-diffusion equation efficiently, where MMOC-Galerkin is conservative locally on every elements and a $3/2$ order error estimates is derived. While lots of mapping integrals of test functions are introduced. The computation becomes more complicated and difficult.

Therefore, we develop and improve substantially the work of Arbogast and Wheeler [2], and put forward a mixed finite element-characteristic mixed element method. This method decreases computational work greatly, and the feasibility and effectiveness is checked experimentally in [29]. Only first order convergence rate is derived and this method could not be generalized for three-dimensional problems. Since finite volume method [4, 19] is carried out simply, could obtain numerical approximations accurately and conservatively, thus it is an effective tool for solving partial differential equations. The method of mixed finite element [15, 16, 25] can solve the pressure and Darcy velocity simultaneously, and develops the accuracy. Combined the above two methods, a mixed finite volume method is discussed in [27, 31, 32] and numerical experiments are argued in [5, 22]. Theoretical analysis is given for elliptic problem in [8-10] and a general discussion frame is given for mixed finite volume method. Rui and Pan [24, 26] use this method to discuss numerical computation for hypotonic oil-gas flow problems. Based on the previous studies, a type of mixed volume element with characteristic mixed volume element method is put forward for three-dimensional underground water pollution problem in this paper. The pressure and Darcy velocity are computed simultaneously by a conservative mixed volume element and the accuracy of Darcy velocity is improved. A conservative characteristic mixed finite volume element is used to compute the concentration, where the convection is approximated along the characteristics and the diffusion is discretized by the mixed volume element. The method of characteristics not only has strong stability without numerical dispersion at sharp fronts, but also has small time truncation errors. In actual computations, a large time step may be adopted and the efficiency is developed without losing accuracy. We apply the method of mixed finite volume element to obtain the concentration and its adjoint vector simultaneously. Take piecewise-defined constants as test functions, then we get the local conservation of mass. Using the theory of a priori estimates of differential equations, we obtain an

optimal order estimates in L^2 norm superior to $3/2$-order in [2]. Finally, the computational efficiency and theoretical results are illustrated experimentally. Thus, the potential is shown to be an efficient tool in solving some actual applications [2, 17, 28, 36].

Some symbols and assumptions are introduced. The regularity conditions of (1.1)-(1.7) are defined by

$$\text{(R)}\quad \begin{cases} p \in L^{\infty}(H^1), \\ \mathbf{u} \in L^{\infty}(H^1(div))\bigcap L^{\infty}(W_{\infty}^1)\bigcap W_{\infty}^1(L^{\infty})\bigcap H^2(L^2), \\ c \in L^{\infty}(H^2)\bigcap H^1(H^1)\bigcap L^{\infty}(W_{\infty}^1)\bigcap H^2(L^2), \\ s \in L^{\infty}(H^2)\bigcap H^2(L^2). \end{cases}$$

Suppose that the coefficients satisfy the following positive definite conditions:

$$\text{(C)}\quad 0 < k_* \le \kappa(c) \le k^*, \quad 0 < \theta_* \le \theta(X) \le \theta^*, \quad 0 < \rho_* \le \rho(X) \le \rho^*,$$

$$0 < D_* \le D(X) \le D^*,$$

where k_*, k^*, θ_*, θ^*, ρ_*, ρ^*, D_*, and D^* are positive constants.

For simplicity, the problem (1.1)-(1.7) is assumed to be Ω-periodic [12, 13, 17, 18, 31], that is, all the functions are Ω-periodic. This assumption seems physically reasonable, since no-flow boundaries are generally treated by reflection, and because interior flow factors are much more important than boundary effects. Thus, the conditions (1.5) possibly is dropped [17, 35, 36].

The paper is organized as follows. In Section 1, mathematical model is stated, and physical background and related research are introduced. In Section 2, some symbols and properties are stated, and two different (coarse and refined) partitions are defined. In Section 3, the authors put forward one method of mixed volume element with characteristic mixed

volume element. A conservative mixed volume element is presented for the flow equation, and the accuracy of Darcy velocity is improved by one-order. The method of characteristic mixed volume element is used to solve the concentration equation, where the convection is treated by the method of characteristics and the diffusion is approximated by the method of mixed volume element. The composite scheme develops the computational stability and accuracy greatly, and the nature of conservation is preserved. It is an important feature in solving such complicated physical problems. The adsorption concentration is solved by the method of lower order finite element. In Section 4, convergence analysis is shown. A second-order error estimates in l^2 norm is obtained, improving the famous convergence rate of $3/2$-order presented by Arbogast and Wheeler. In Section 5, a mixed volume element with characteristic mixed volume element method is discussed. In the applications, a large step could be adopted for the flow equation, then it could shorten the computational scale and possibly decreases time cost. In Section 6, two numerical experiments are illustrated to support theoretical results, and numerical data confirm that the method is applicable and efficient in actual applications.

In this paper, let K and ε denote a generic positive constant and a generic small positive number, respectively. They may have different definitions at different places.

2. Notation and Preparations

Here two different partitions are defined for showing the numerical composite scheme. The first partition with a large step is nonuniform for solving the pressure and Darcy velocity, and the second nonuniform one is for the concentration. For simplicity, take $\Omega = \{[0, 1]\}^3$ and let $\partial\Omega$ denote the boundary. The first partition is defined by $\delta_x \times \delta_y \times \delta_z$,

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

$$\delta_y : 0 = y_{1/2} < y_{3/2} < \cdots < y_{N_y-1/2} < y_{N_y+1/2} = 1,$$

$$\delta_z : 0 = z_{1/2} < z_{3/2} < \cdots < z_{N_z-1/2} < z_{N_z+1/2} = 1.$$

For $i = 1, 2, \cdots, N_x$, $j = 1, 2, \cdots, N_y$, $k = 1, 2, \cdots, N_z$, define $\Omega_{ijk} = \{(x, y, z) : x_{i-1/2} < x < x_{i+1/2}, y_{j-1/2} < y < y_{j+1/2}, z_{k-1/2} < z < z_{k+1/2}\}$, $x_i = (x_{i-1/2} + x_{i+1/2})/2$, $y_j = (y_{j-1/2} + y_{j+1/2})/2$, $z_k = (z_{k-1/2} + z_{k+1/2})/2$, $h_{x_i} = x_{i+1/2} - x_{i-1/2}$, $h_{y_j} = y_{j+1/2} - y_{j-1/2}$, $h_{z_k} = z_{k+1/2} - z_{k-1/2}$, $h_{x,i+1/2} = (h_{x_i} + h_{x_{i+1}})/2 = x_{i+1} - x_i$, $h_{y,j+1/2} = (h_{y_j} + h_{y_{j+1}})/2 = y_{j+1} - y_j$, $h_{z,k+1/2} = (h_{z_k} + h_{z_{k+1}})/2 = z_{k+1} - z_k$. Define $h_x = \max\limits_{1\le i\le N_x}\{h_{x_i}\}$, $h_y = \max\limits_{1\le j\le N_y}\{h_{y_j}\}$, $h_z = \max\limits_{1\le k\le N_z}\{h_{z_k}\}$, and $h_p = (h_x^2 + h_y^2 + h_z^2)^{1/2}$. The partition is regular if there exist two constants $\alpha_1 > 0$ and $\alpha_2 > 0$ such that

$$\min_{1\le i\le N_x}\{h_{x_i}\} \ge \alpha_1 h_x,\ \min_{1\le j\le N_y}\{h_{y_j}\} \ge \alpha_1 h_y,\ \min_{1\le k\le N_z}\{h_{z_k}\} \ge \alpha_1 h_z,$$

$$\min\{h_x, h_y, h_z\} \ge \alpha_2 \max\{h_x, h_y, h_z\}.$$

Here α_1 and α_2 depend on $\delta_x \times \delta_y \times \delta_z$. A simplified case with $N_x = 4$, $N_y = 3$ and $N_z = 3$ is illustrated in Figure 1. Introduce $M_l^d(\delta_x) = \{f \in C^l[0, 1] : f|_{\Omega_i} \in p_d(\Omega_i), i = 1, 2, \cdots, N_x\}$ as an experimental space, where $p_d(\Omega_i)$ denotes a space consisting of all the polynomial functions of degree at most d on $\Omega_i = [x_{i-1/2}, x_{i+1/2}]$, f is possibly discontinuous on $[0, 1]$ as $l = -1$, $M_l^d(\delta_y)$ and $M_l^d(\delta_z)$ are defined similarly. Let $S_h = M_{-1}^0(\delta_x) \otimes M_{-1}^0(\delta_y) \otimes M_{-1}^0(\delta_z)$, $V_h = \{\mathbf{w} | \mathbf{w} = (w^x, w^y, w^z), w^x \in M_0^1(\delta_x) \otimes M_{-1}^0(\delta_y) \otimes M_{-1}^0(\delta_z), w^y \in M_{-1}^0(\delta_x) \otimes M_0^1(\delta_y) \otimes M_{-1}^0(\delta_z), w^z \in M_{-1}^0(\delta_x) \otimes M_{-1}^0(\delta_y) \otimes M_0^1(\delta_z), \mathbf{w} \cdot \gamma|_{\partial\Omega} = 0\}$. 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 $v(x_i, y_j, z_k)$, $v(x_{i+1/2}, y_j, z_k)$, $v(x_i, y_{j+1/2}, z_k)$ and $v(x_i, y_j, z_{k+1/2})$, respectively.

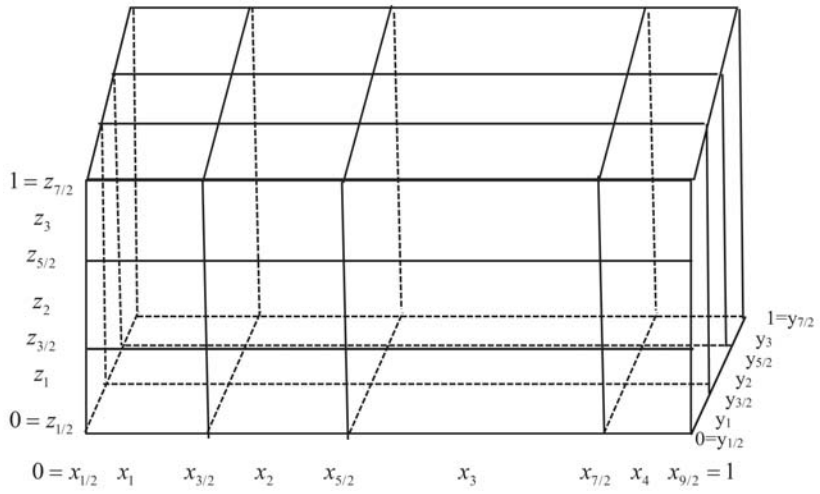

Figure 1. Nonuniform partition.

The inner products and norms are defined as follows:

$$(v,\, w)_m = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x_i} h_{y_j} h_{z_k} v_{ijk} w_{ijk},\ (v,\, w)_x$$

$$= \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x_{i-1/2}} h_{y_j} h_{z_k} v_{i-1/2,\, jk} w_{i-1/2,\, jk},$$

$$(v,\, w)_y = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x_i} h_{y_{j-1/2}} h_{z_k} v_{i,\, j-1/2,\, k} w_{i,\, j-1/2,\, k},$$

$$(v,\, w)_z = \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\sum_{k=1}^{N_z} h_{x_i} h_{y_j} h_{z_{k-1/2}} v_{ijk-1/2} w_{ij,\, k-1/2},$$

$$\|v\|_s^2 = (v,\, v)_s,\ s = m,\, x,\, y,\, z, \quad \|v\|_\infty = \max_{1\le i\le N_x, 1\le j\le N_y, 1\le k\le N_z} |v_{ijk}|,$$

$$\|v\|_{\infty(x)} = \max_{1\le i\le N_x, 1\le j\le N_y, 1\le k\le N_z} |v_{i-1/2,\, jk}|,$$

$$\|v\|_{\infty(y)} = \max_{1\le i\le N_x,1\le j\le N_y,1\le k\le N_z} |v_{i,\,j-1/2,\,k}|,$$

$$\|v\|_{\infty(z)} = \max_{1\le i\le N_x,1\le j\le N_y,1\le k\le N_z} |v_{ij,\,k-1/2}|.$$

For a vector $\mathbf{w} = (w^x,\, w^y,\, w^z)^T$, let

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

$$\|\mathbf{w}\|_m = (\|w^x\|_m^2 + \|w^y\|_m^2 + \|w^z\|_m^2)^{1/2},\ \|\mathbf{w}\|_\infty = \|w^x\|_\infty + \|w^y\|_\infty + \|w^z\|_\infty.$$

Define $W_p^m(\Omega) = \{v \in L^p(\Omega) | \dfrac{\partial^n v}{\partial x^{n-l-r}\partial y^l \partial z^r} \in L^p(\Omega),\ n-l-r \ge 0,$ $l = 0, 1, \cdots, n;\ r = 0, 1, \cdots, n,\ n = 0, 1, \cdots, m;\ 0 < p < \infty\}$ and let $H^m(\Omega) = W_2^m(\Omega)$. The inner products and norms in $L^2(\Omega)$ are denoted by $(\cdot, \cdot)$ and $\|\cdot\|$. It is easy to see that

$$\|v\|_m = \|v\|, \quad v \in S_h. \tag{2.1}$$

The difference operators and other notation are introduced,

$$[d_x v]_{i+1/2,\,jk} = \frac{v_{i+1,\,jk} - v_{ijk}}{h_{x,\,i+1/2}}, \quad [d_y v]_{i,\,j+1/2,\,k} = \frac{v_{i,\,j+1,\,k} - v_{ijk}}{h_{y,\,j+1/2}},$$

$$[d_z v]_{ij,\,k+1/2} = \frac{v_{ij,\,k+1} - v_{ijk}}{h_{z,\,k+1/2}};$$

$$[D_x w]_{ijk} = \frac{w_{i+1/2,\,jk} - w_{i-1/2,\,jk}}{h_{x_i}}, \quad [D_y w]_{ijk} = \frac{w_{i,\,j+1/2,\,k} - w_{i,\,j-1/2,\,k}}{h_{y_j}},$$

$$[D_z w]_{ijk} = \frac{w_{ij,\,k+1/2} - w_{ij,\,k-1/2}}{h_{z_k}};$$

$$\hat{w}^x_{ijk} = \frac{w^x_{i+1/2,\,jk} + w^x_{i-1/2,\,jk}}{2},\ \hat{w}^y_{ijk} = \frac{w^y_{i,\,j+1/2,\,k} + w^y_{i,\,j-1/2,\,k}}{2},$$

$$\hat{w}^z_{ijk} = \frac{w^z_{ij,\,k+1/2} + w^z_{ij,\,k-1/2}}{2},$$

$$\overline{w}^x_{ijk} = \frac{h_{x,\,i+1}}{2h_{x,\,i+1/2}} w_{ijk} + \frac{h_{x,\,i}}{2h_{x,\,i+1/2}} w_{i+1,\,jk},$$

$$\overline{w}^y_{ijk} = \frac{h_{y,\,j+1}}{2h_{y,\,j+1/2}} w_{ijk} + \frac{h_{y,\,j}}{2h_{y,\,j+1/2}} w_{i,\,j+1,\,k},$$

$$\overline{w}^z_{ijk} = \frac{h_{z,\,k+1}}{2h_{z,\,k+1/2}} w_{ijk} + \frac{h_{z,\,k}}{2h_{z,\,k+1/2}} w_{ij,\,k+1},$$

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

The properties are prepared for the following numerical analysis.

Lemma 1. *For* $v \in S_h$ *and* $\mathbf{w} \in V_h$,

$$(v,\, D_x w^x)_m = -(d_x v,\, w^x)_x,\ (v,\, D_y w^y)_m$$

$$= -(d_y v,\, w^y)_y,\ (v,\, D_z w^z)_m = -(d_z v,\, w^z)_z. \tag{2.2}$$

Lemma 2. *For* $\mathbf{w} \in V_h$,

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

Proof. In fact, it is necessary to prove $\|\hat{w}^x\|_m \le \|w^x\|_x$, $\|\hat{w}^y\|_m \le \|w^y\|_y$, and $\|\hat{w}^z\|_m \le \|w^z\|_z$. Note that

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

then we have $\|\hat{w}^x\|_m \le \|w^x\|_x$, and get the other two inequalities.

Lemma 3. *For* $q \in S_h$,

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

where M is a constant independent of q and h.

Lemma 4. *For* $\mathbf{w} \in V_h$,

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

Proof. Here we only discuss $\|w^x\|_x \le \|D_x w^x\|_m$. From the fact that

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

and by the Cauchy inequality, we have

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

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

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

Then the proof of Lemma 4 is completed.

Another partition is obtained by refining the coarse partition of $\Omega = \{[0, 1]\}^3$ uniformly. Generally, we take the step by $h_c = h_p / 2$ or $h_p / 4$.

Since the absorption concentration changes slow and stably, Equation (1.2) is discussed on the first partition. A first-order finite element space M_h is constructed on a hexahedron element $\Omega_{ijk} = [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}] \times [z_{k-1/2}, z_{k+1/2}]$ seen in [7, 20].

3. The Procedures of Mixed Finite Volume Element with Modified Characteristic Mixed Volume Element

3.1. The procedures

In order to use the mixed finite volume element, we rewrite Equation (1.1) in a normalized formulation

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

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

For Equation (1.2), considering that the flow transports along the characteristic direction, thus we apply the method of characteristics to approximate the first-order hyperbolic term. The computational algorithm could use a large time step and has the strong stability and high order accuracy. Let $\psi(X, \mathbf{u}) = [\theta^2(X) + |\mathbf{u}|^2]^{1/2}$, $\frac{\partial}{\partial \tau} = \psi^{-1}\{\theta \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\}$.

Equation (1.2) is rewritten as follows for applying the method of mixed volume element,

$$\psi \frac{\partial c}{\partial \tau} + \rho \frac{\partial s}{\partial t} + \nabla \cdot \mathbf{g} = f(X, c), \tag{3.2a}$$

$$\mathbf{g} = -\theta D \nabla c, \tag{3.2b}$$

where $f(X, c) = -qc$.

Let P, $\mathbf{U}$, C, $\mathbf{G}$ and S denote the discrete solutions of p, $\mathbf{u}$, c, $\mathbf{g}$ and s, respectively. The pressure and Darcy velocity are computed by the method of characteristic mixed volume element,

$$(D_x U^{x,n+1} + D_y U^{y,n+1} + D_z U^{z,n+1}, v)_m = (q^{n+1}, v)_m, \quad \forall v \in S_h, \tag{3.3a}$$

$$\begin{aligned}(k^{-1}(\overline{C}^{x,n})U^{x,n+1}, w^x)_x &+ (k^{-1}(\overline{C}^{y,n})U^{y,n+1}, w^y)_y \\ &+ (k^{-1}(\overline{C}^{z,n})U^{z,n+1}, w^z)_z \\ &- (P^{n+1}, D_x w^x + D_x w^y + D_x w^z)_m = 0, \quad \forall \mathbf{w} \in V_h.\end{aligned} \tag{3.3b}$$

The derivative along the characteristics in (3.2a) is approximated by the backward difference quotient

$$\frac{\partial c^{n+1}}{\partial \tau} \approx \frac{c^{n+1} - c^n(X - \theta^{-1}\mathbf{u}^{n+1}(X)\Delta t)}{\Delta t(1 + \theta^{-2}|\mathbf{u}^{n+1}|^2)^{1/2}}.$$

Equation (3.2) is discretized by the characteristic mixed volume element method

$$\begin{aligned}\left(\theta \frac{C^{n+1} - \hat{C}^n}{\Delta t}, v\right)_m + \left(\rho \frac{S^{n+1} - S^n}{\Delta t}, v\right)_m &+ (D_x G^{x,n+1} + D_y G^{y,n+1} \\ &+ D_z G^{z,n+1}, v)_m = (f(\hat{C}^n), v)_m, \ \forall v \in S_h,\end{aligned} \tag{3.4a}$$

$$\begin{aligned}(D^{-1}G^{x,n+1}, w^x)_x + (D^{-1}G^{y,n+1}, w^y)_y + (D^{-1}G^{z,n+1}), w^z)_z \\ - (C^{n+1}, D_x w^x + D_y w^y + D_z w^z)_m = 0, \ \forall \mathbf{w} \in V_h,\end{aligned} \tag{3.4b}$$

where $\hat{C}^n = C^n(\hat{X}^n)$, $\hat{X}^n = X - \theta^{-1}\mathbf{U}^{n+1}\Delta t$.

The adsorption concentration changes slow and stably with respect to t, so we obtain an explicit scheme to approximate Equation (1.3),

$$\left(\frac{S^{n+1}-S^n}{\Delta t},\ \varphi\right) = \hat{\alpha}(\phi(C^n)-S^n,\ \varphi), \quad \varphi \in M_h. \tag{3.5}$$

Initial approximations are defined by

$$C^0 = \widetilde{C}^0, \quad \mathbf{G}^0 = \widetilde{\mathbf{G}}^0, \quad S^0 = \widetilde{S}^0, \quad X \in \Omega, \tag{3.6}$$

where $(\widetilde{C}^0, \widetilde{\mathbf{G}}^0)$ is the elliptic projection of $(c_0, \mathbf{g}_0)$, and $\widetilde{S}^0$ is an L^2 projection of s_0 (see the definitions in the next section).

The composite procedures run as follows. First of all, the elliptic projection and the initial values are used to obtain $\{\widetilde{C}^0, \widetilde{\mathbf{G}}^0\}$, as the initial approximations of c_0 and $\mathbf{g}_0 = -\theta D\nabla c_0$, i.e., $C^0 = \widetilde{C}^0$, $\mathbf{G}^0 = \widetilde{\mathbf{G}}^0$. Use s_0 and the L^2 projection to get $S^0 = \widetilde{S}^0$. Secondly, S^1 is computed by (3.5). Then, $\{\mathbf{U}^1, P^1\}$ is computed by the method of conjugate gradient and mixed volume element (3.3). Similarly, $\{C^1, \mathbf{G}^1\}$ is obtained by (3.4). Next, S^2, $\{\mathbf{U}^2, P^2\}$ and $\{C^2, \mathbf{G}^2\}$ are computed by (3.4), (3.3), and (3.5). The computations proceed repeatedly and all the numerical solutions are obtained. By the positive definite condition (C), the solutions exist and are unique.

3.2. Local and whole conservation of mass

Assume that the problem (1.1)-(1.7) has no source or sink, i.e., $q \equiv 0$, and assume that the boundary condition is impermeable. Here we ignore the effect of adsorption. Thus, for simplicity we take $l = 1$, or suppose that two partitions are the same. On every element $J_c \subset \Omega$, $J_c = \Omega_{ijk} = [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}] \times [z_{k-1/2}, z_{k+1/2}]$, the local conservation of mass is interpreted for Equation (1.2) by

$$\int_{J_c} \psi \frac{\partial c}{\partial \tau} dX - \int_{\partial J_c} \mathbf{g} \cdot \gamma_{J_c} dS = 0, \tag{3.7}$$

∂J_c denotes the boundary of J_c and γ_{J_c} denotes its outer normal vector. Then, the discrete local conservation holds for Equation (3.4a).

Theorem 1. *If* $q \equiv 0$, *and the factor of surface absorption is ignored, then on every element* $J_c \subset \Omega$, (3.4a) *satisfies the conservation law*

$$\int_{J_c} \theta \frac{C^{n+1} - \hat{C}^n}{\Delta t} dX - \int_{\partial J_c} \mathbf{G}^{n+1} \cdot \gamma_{J_c} dS = 0. \tag{3.8}$$

Proof. Note that $v = \begin{cases} 1, & J_c = \Omega_{ijk}, \\ 0, & \text{otherwise}, \end{cases}$ $v \in S_h$. Then, (3.4a) turns into

$$\left(\theta \frac{C^{n+1} - \hat{C}^n}{\Delta t}, 1 \right)_{\Omega_{ijk}} + (D_x G^{x,n+1} + D_y G^{y,n+1} + D_z G^{z,n+1}, 1)_{\Omega_{ijk}} = 0. \tag{3.9}$$

Using the previous notation, we have

$$\left(\theta \frac{C^{n+1} - \hat{C}^n}{\Delta t}, 1 \right)_{\Omega_{ijk}} = \theta_{ijk} \left(\frac{C_{ijk}^{n+1} - \hat{C}_{ijk}^n}{\Delta t} \right) h_{x_i} h_{y_j} h_{z_k} = \int_{\Omega_{ijk}} \theta \frac{C^{n+1} - \hat{C}^n}{\Delta t} dX, \tag{3.10a}$$

$$\begin{aligned} (D_x G^{x,n+1} + D_y G^{y,n+1} + D_z G^{z,n+1}, 1)_{\Omega_{ijk}} &= (G_{i+1/2,jk}^{x,n+1} - G_{i-1/2,jk}^{x,n+1}) h_{y_j} h_{z_k} \\ &+ (G_{i,j+1/2,k}^{y,n+1} - G_{i,j-1/2,k}^{y,n+1}) h_{x_i} h_{z_k} + (G_{ij,k+1/2}^{z,n+1} - G_{ij,k-1/2}^{z,n+1}) h_{x_i} h_{y_j} \\ &= - \int_{\partial \Omega_{ijk}} \mathbf{G}^{n+1} \cdot \gamma_{J_c} dS. \end{aligned} \tag{3.10b}$$

Substituting (3.10) into (3.9), we could complete this proof.

Furthermore, we get the conservation of mass on the whole domain.

Theorem 2. *Suppose* $q \equiv 0$ *and the boundary is impermeable. The factor of surface absorption is ignored. Then,*

$$\int_{\Omega} \theta \frac{C^{n+1} - \hat{C}^n}{\Delta t} dX = 0, \; n \geq 0. \tag{3.11}$$

Proof. Summing (3.8) on all the elements, we have

$$\sum_{i,j,k} \int_{\Omega_{ijk}} \theta \frac{C^{n+1} - \hat{C}^n}{\Delta t} dX - \sum_{i,j,k} \int_{\partial\Omega_{ijk}} \mathbf{G}^{n+1} \cdot \gamma_{J_c} dS = 0. \tag{3.12}$$

Then, the proof is completed by using $-\sum_{i,j,k} \int_{\partial\Omega_{ijk}} \mathbf{G}^{n+1} \cdot \gamma_{J_c} dS = -\int_{\partial\Omega} \mathbf{G}^{n+1} \cdot \gamma dS = 0$.

4. Convergence Analysis

The elliptic projections are introduced first. $\widetilde{\mathbf{U}} \in V_h$ and $\widetilde{P} \in S_h$ are defined by

$$(D_x\widetilde{U}^x + D_y\widetilde{U}^y + D_z\widetilde{U}^z, v)_m = (q, v)_m, \; \forall v \in S_h, \tag{4.1a}$$

$$(k^{-1}(c)\widetilde{U}^x, w^x)_x + (k^{-1}(c)\widetilde{U}^y, w^y)_y + (k^{-1}(c)\widetilde{U}^z, w^z)_z - (\widetilde{P}, D_x w^x + D_y w^y + D_z w^z)_m = 0, \; \forall \mathbf{w} \in V_h, \tag{4.1b}$$

where c denotes the exact solution of (1.1)-(1.7).

Let $F = f - \psi \frac{\partial c}{\partial \tau} - \rho \frac{\partial s}{\partial t}$. Define $\widetilde{\mathbf{G}} \in V_h$, $\widetilde{C} \in S_h$ by

$$(D_x\widetilde{G}^x + D_y\widetilde{G}^y + D_z\widetilde{G}^z, v)_m = (F, v)_m, \; \forall v \in S_h, \tag{4.2a}$$

$$(D^{-1}\widetilde{G}^x, w^x)_x + (D^{-1}\widetilde{G}^y, w^y)_y + (D^{-1}\widetilde{G}^z, w^z)_z - (\widetilde{C}, D_x w^x + D_y w^y + D_z w^z)_m = 0, \; \forall \mathbf{w} \in V_h. \tag{4.2b}$$

The L^2 finite element projection $\widetilde{S} \in M_h$ is defined by

$$(S, z) = (s, z), \quad \forall z \in M_h. \tag{4.3}$$

Let $\pi = P - \widetilde{P}$, $\eta = \widetilde{P} - p$, $\sigma = \mathbf{U} - \widetilde{\mathbf{U}}$, $\rho = \widetilde{\mathbf{U}} - \mathbf{u}$, $\xi = C - \widetilde{C}$, $\zeta = \widetilde{C} - c$, $\alpha = \mathbf{G} - \widetilde{\mathbf{G}}$, $\beta = \widetilde{\mathbf{G}} - \mathbf{g}$, $\mu = S - \widetilde{S}$, and $\lambda = \widetilde{S} - s$. Suppose that (1.1)-(1.7) satisfies the positive definite condition (C), and suppose that exact solutions satisfy the regularity (R). From the discussions of Weiser and Wheeler [32], we see that auxiliary functions $\{\widetilde{\mathbf{U}}, \widetilde{P}, \widetilde{\mathbf{G}}, \widetilde{C}\}$ of (4.1) and (4.2) exist and are unique.

Lemma 5. *If the coefficients and exact solutions of* (1.1)-(1.7) *satisfy* (C) *and* (R), *then there exist two constants* $\overline{C}_1 > 0$ *and* $\overline{C}_2 > 0$ *independent of h such that*

$$\|\eta\|_m + \|\zeta\|_m + \|\|\rho\|\| + \|\|\beta\|\| + \left\|\frac{\partial \eta}{\partial t}\right\|_m + \left\|\frac{\partial \zeta}{\partial t}\right\|_m \le \overline{C}_1\{h_p^2 + h_c^2\}, \tag{4.4a}$$

$$\left\|\|\widetilde{\mathbf{U}}\|\right\|_\infty + \left\|\|\widetilde{\mathbf{G}}\|\right\|_\infty \le \overline{C}_2. \tag{4.4b}$$

Under the same assumptions, using the property of L^2 projection [7, 20], we have the following estimates.

Lemma 6. *Suppose that the adsorption concentration satisfies the regularity* (R). *Then there exists a constant* $\overline{C}_3 > 0$ *independent of* h_c *such that*

$$\|\lambda\|_{L^2} + \left\|\frac{\partial \lambda}{\partial t}\right\|_{L^2} \le \overline{C}_3 h_c^2, \tag{4.5}$$

π *and* σ *are estimated first. Subtracting* (4.1a) $(t = t^{n+1})$ *and* (4.1b) $(t = t^{n+1})$, *respectively from* (3.3a) *and* (3.3b), *we have*

$$(D_x\sigma^{x,n+1} + D_y\sigma^{y,n+1} + D_z\sigma^{z,n+1}, v)_m = 0, \ \forall v \in S_h, \tag{4.6a}$$

$$(k^{-1}(\overline{C}^{x,n})\sigma^{x,n+1},\ w^x)_x + (k^{-1}(\overline{C}^{y,n})\sigma^{y,n+1},\ w^y)_y + (k^{-1}(\overline{C}^{z,n})\sigma^{z,n+1},\ w^z)_z$$

$$-(\pi^{n+1},\ D_x w^x + D_y w^y + D_z w^z)_m = -\Big\{\Big((k^{-1}(\overline{C}^{x,n}) - k^{-1}(c^{n+1}))\widetilde{U}^{x,n+1},\ w^x\Big)_x$$

$$+\Big((k^{-1}(\overline{C}^{y,n}) - k^{-1}(c^{n+1}))\widetilde{U}^{y,n+1},\ w^y\Big)_y + \Big((k^{-1}(\overline{C}^{z,n}) - k^{-1}(c^{n+1}))\widetilde{U}^{z,n+1},\ w^z\Big)_z\Big\},$$

$$\forall \mathbf{w} \in V_h. \qquad (4.6b)$$

Take $v = \pi^{n+1}$ in (4.6a), $\mathbf{w} = \sigma^{n+1}$ in (4.6b), and combine them together, we have

$$(k^{-1}(\overline{C}^{x,n})\sigma^{x,n+1},\ \sigma^{x,\,n+1})_x + (k^{-1}(\overline{C}^{y,n})\sigma^{y,n+1},\ \sigma^{y,\,n+1})_y + (k^{-1}(\overline{C}^{z,n})\sigma^{z,n+1},$$

$$\sigma^{z,\,n+1})_z = -\sum_{s=x,\ y,\ z}((k^{-1}(\overline{C}^{s,n}) - k^{-1}(c^{n+1}))\widetilde{U}^{s,n+1},\ \sigma^{s,n+1})_s. \qquad (4.7)$$

Equation (4.7) is estimated by using Lemma 1-Lemma 5, the Taylor expansion and (C),

$$|||\sigma^{n+1}|||^2 \le K\sum_{s=x,\ y,\ z}\|\overline{C}^{s,n} - c^{n+1}\|_m^2$$

$$\le K\left\{\sum_{s=x,\ y,\ z}\left\|\widetilde{C}^{s,n} - c^n\right\|_m^2 + \|\xi^n\|_m^2 + \|\zeta^n\|_m^2 + (\Delta t)^2\right\} \le K\left\{\|\xi^n\|^2 + h_c^4 + (\Delta t)^2\right\}.$$

(4.8)

$\pi^{n+1} \in S_h$ is discussed by using the method of duality [20, 23] later. Consider the following elliptic problem:

$$\nabla \cdot \omega = \pi^{n+1},\ X = (x,\ y,\ z)^T \in \Omega, \qquad (4.9a)$$

$$\omega = \nabla p,\ X \in \Omega, \qquad (4.9b)$$

$$\omega \cdot \gamma = 0,\ X \in \partial\Omega. \qquad (4.9c)$$

Using the regularity (4.9),

$$\sum_{s=x,\ y,\ z}\left\|\frac{\partial \omega^s}{\partial s}\right\|_m^2 \le K\|\pi^{n+1}\|_m^2. \qquad (4.10)$$

If $\tilde{\omega} \in V_h$ satisfies

$$\left(\frac{\partial \tilde{\omega}^s}{\partial s}, v\right)_m = \left(\frac{\partial \omega^s}{\partial s}, v\right)_m, \ \forall v \in S_h, \ s = x, y, z, \tag{4.11a}$$

then the solution $\tilde{\omega}$ exists and is estimated by

$$\sum_{s=x,y,z} \left\| \frac{\partial \tilde{\omega}^s}{\partial s} \right\|_m^2 \le \sum_{s=x,y,z} \left\| \frac{\partial \omega^s}{\partial s} \right\|_m^2. \tag{4.11b}$$

Using Lemma 4, (4.9), (4.10) and (4.6), we have

$$\begin{aligned} \|\pi^{n+1}\|_m^2 &= (\pi^{n+1}, \nabla \cdot \omega) = (\pi^{n+1}, D_x\tilde{\omega}^x + D_y\tilde{\omega}^y + D_z\tilde{\omega}^z)_m \\ &= \sum_{s=x,y,z} (k^{-1}(\overline{C}^{s,n})\sigma^{s,n+1}, \tilde{\omega}^s)_s + \sum_{s=x,y,z} ((k^{-1}(\overline{C}^{s,n}) - k^{-1}(c^{n+1}))\tilde{U}^{s,n+1}, \tilde{\omega}^s)_s \\ &\le K|||\tilde{\omega}||| \left\{ |||\sigma^{n+1}|||^2 + \|\xi^n\|_m^2 + h_c^4 + (\Delta t)^2 \right\}^{1/2}. \end{aligned} \tag{4.12}$$

From Lemma 4, (4.10) and (4.11), we have

$$|||\tilde{\omega}|||^2 \le \sum_{s=x,y,z} \|D_s\tilde{\omega}^s\|_m^2 = \sum_{s=x,y,z} \left\| \frac{\partial \tilde{\omega}^s}{\partial s} \right\|_m^2 \le \sum_{s=x,y,z} \left\| \frac{\partial \omega^s}{\partial s} \right\|_m^2 \le K\|\pi^{n+1}\|_m^2. \tag{4.13}$$

Substituting (4.13) into (4.12),

$$\|\pi^{n+1}\|_m^2 \le K\{|||\sigma^{n+1}|||^2 + \|\xi^n\|_m^2 + h_c^4 + (\Delta t)^2\} \le K\{\|\xi^n\|_m^2 + h_c^4 + (\Delta t)^2\}. \tag{4.14}$$

Error function μ is discussed later. It follows from (1.3) $(t = t^{n+1})$, (3.5) and (4.3),

$$\begin{aligned} \left(\frac{\mu^{n+1} - \mu^n}{\Delta t}, \varphi\right) &= \hat{\alpha}(\phi(C^n) - \phi(\tilde{C}^n) + \phi(\tilde{C}^n) - \phi(C^{n+1}), \varphi) - \hat{\alpha}(\theta^n, \varphi) \\ &\quad - \hat{\alpha}(S^{n+1} - S^n, \varphi) - \left(\frac{\partial \tilde{s}^{n+1}}{\partial t} - \frac{s^{n+1} - s^n}{\Delta t}, \varphi\right), \ \forall \varphi \in M_h. \end{aligned} \tag{4.15}$$

For the Langmuir isotherm, it is easy to see that $\phi'(c) \le k_1$ holds from $\phi(c) = \dfrac{k_1 c}{1 + k_2 c}$ and $\phi'(c) = \dfrac{k_1}{(1 + k_2 c)^2}$. For the Freundlinch isotherm, $\phi(c) = k_3 c^p$, $\phi'(c) = k_3 p c^{p-1}$, let $p = 1$, then $f'(c) \le k_3$. The analysis proceeds by applying the Lagrange mean value theorem. Taking $\varphi = \partial_t \mu^n = \dfrac{\mu^{n+1} - \mu^n}{\Delta t}$ in (4.15), using Lemma 5, Lemma 6 and the regularity (R), we have

$$\|\partial_t \mu^n\|_{L^2}^2 \le K \left\{ \|\xi^n\|_{L^2}^2 + \|\mu^n\|_{L^2}^2 + h_c^4 + h_p^4 + (\Delta t)^2 \right\}. \tag{4.16a}$$

Taking $\varphi = \mu^{n+1}$ in (4.15), we have

$$\frac{1}{2\Delta t} \{ \|\mu^{n+1}\|_{L^2}^2 - \|\mu^n\|_{L^2}^2 \} \le K \{ \|\mu^{n+1}\|_{L^2}^2 + \|\mu^n\|_{L^2}^2 + \|\xi^n\|_{L^2}^2 + h_c^4 + h_p^4 + (\Delta t)^2 \}. \tag{4.16b}$$

Next, Equation (1.2) is estimated. Subtracting (4.2a) and (4.2b) $t = t^{n+1}$, respectively from (3.4a) and (3.4b), and taking $v = \xi^{n+1}$ and $w = \alpha^{n+1}$, we have

$$\left(\theta \frac{C^{n+1} - \hat{C}^n}{\Delta t}, \xi^{n+1} \right)_m + \left(\rho \frac{C'^{n+1} - C'^n}{\Delta t}, \xi^{n+1} \right)_m + (D_x \alpha^{x, n+1} + D_y \alpha^{y, n+1} + D_z \alpha^{z, n+1}, \xi^{n+1})_m = \left(f(\hat{C}^n) - f(c^{n+1}) + \psi^{n+1} \frac{\partial c^{n+1}}{\partial \tau} + \rho \frac{\partial c'^{n+1}}{\partial t}, \xi^{n+1} \right)_m, \tag{4.17a}$$

$$(D^{-1} \alpha^{x, n+1}, \alpha^{x, n+1})_x + (D^{-1} \alpha^{y, n+1}, \alpha^{y, n+1})_y + (D^{-1} \alpha^{z, n+1}), \alpha^{z, n+1})_z - (\xi^{n+1}, D_x \alpha^{x, n+1} + D_y \alpha^{y, n+1} + D_z \alpha^{z, n+1})_m = 0. \tag{4.17b}$$

Considering the sum of (4.17a) and (4.17b),

$$\left(\theta\frac{C^{n+1}-\hat{C}^n}{\Delta t},\,\xi^{n+1}\right)_m+\left(\rho\frac{C'^{n+1}-C'^n}{\Delta t},\,\xi^{n+1}\right)_m+(D^{-1}\alpha^{x,n+1},\,\alpha^{x,n+1})_x$$
$$+(D^{-1}\alpha^{y,n+1},\,\alpha^{y,n+1})_y+(D^{-1}\alpha^{z,n+1},\;\;\alpha^{z,n+1})_z$$
$$=\left(f(\hat{C}^n)-f(c^{n+1})+\psi^{n+1}\frac{\partial c^{n+1}}{\partial\tau}+\rho\frac{\partial c'^{n+1}}{\partial t},\,\xi^{n+1}\right)_m. \tag{4.18}$$

Subtracting (1.2) $t=t^{n+1}$ from (4.18), we get the error equation

$$\left(\theta\frac{\xi^{n+1}-\xi^n}{\Delta t},\,\xi^{n+1}\right)_m+\sum_{s=x,\,y,\,z}(D^{-1}\alpha^{s,n+1},\,\alpha^{s,n+1})_s$$
$$=-\left(\rho\frac{\mu^{n+1}-\mu^n}{\Delta t},\,\xi^{n+1}\right)_m+\left(\rho(\frac{\partial s^{n+1}}{\partial t}-\frac{s^{n+1}-s^n}{\Delta t}),\,\xi^{n+1}\right)_m-(\rho\partial_t\lambda^n,\,\xi^n)$$
$$+\left(\left[\theta\frac{\partial c^{n+1}}{\partial t}+\mathbf{u}^{n+1}\cdot\nabla c^{n+1}\right]-\theta\frac{c^{n+1}-\check{c}^{\,n}}{\Delta t},\,\xi^{n+1}\right)_m+\left(\theta\frac{\zeta^{n+1}-\zeta^n}{\Delta t},\,\xi^{n+1}\right)_m$$
$$+(f(\hat{C}^n)-f(c^{n+1}),\,\xi^{n+1})+\left(\theta\frac{\hat{c}^n-\check{c}^{\,n}}{\Delta t},\,\xi^{n+1}\right)_m-\left(\theta\frac{\hat{\zeta}^n-\check{\zeta}^n}{\Delta t},\,\xi^{n+1}\right)_m$$
$$+\left(\theta\frac{\hat{\xi}^n-\check{\xi}^n}{\Delta t},\,\xi^{n+1}\right)_m-\left(\theta\frac{\hat{\zeta}^n-\zeta^n}{\Delta t},\,\xi^{n+1}\right)_m+\left(\theta\frac{\check{\xi}^n-\xi^n}{\Delta t},\,\xi^{n+1}\right)_m, \tag{4.19}$$

where $\check{c}^{\,n}=c^n(X-\theta^{-1}\mathbf{u}^{n+1}\Delta t)$, $\hat{c}^n=c^n(X-\theta^{-1}\mathbf{U}^{n+1}\Delta t)$, $\cdots$.

The inequality $a(a-b)\geq\frac{1}{2}(a^2-b^2)$ is used to estimate the left-hand term of (4.19). The terms on the right-hand side are denoted by $T_1,\,T_2,\,\cdots,\,T_{11}$. Then,

$$\frac{1}{2\Delta t}\{(\theta\xi^{n+1},\,\xi^{n+1})_m-(\theta\xi^n,\,\xi^n)_m\}+\sum_{s=x,\,y,\,z}(D^{-1}\alpha^{s,n+1},\,\alpha^{s,n+1})_s\leq\sum_{i=1}^{11}T_i. \tag{4.20}$$

T_1, T_2, and T_3 of (4.20) are estimated by using the relation of continuous L^2-norm and discrete m-norm [14, 25] and (4.16),

$$|T_1 + T_2 + T_3| \le K\|\partial_t \mu^n\|_m^2 + K\left\{\|\xi^{n+1}\|_m^2 + h_c^4 + (\Delta t)^2\right\}$$
$$\le K\left\{\|\xi^{n+1}\|_m^2 + \|\xi^n\|_m^2 + \|\mu^n\|_m^2 + h_c^4 + h_p^4 + (\Delta t)^2\right\}. \tag{4.21}$$

Noting that $\theta\dfrac{\partial c^{n+1}}{\partial t} + \mathbf{u}^{n+1}\cdot\nabla c^{n+1} = \psi^{n+1}\dfrac{\partial c^{n+1}}{\partial \tau}$, we have

$$\frac{\partial c^{n+1}}{\partial \tau} - \frac{\theta}{\psi^{n+1}}\frac{c^{n+1} - \check{c}^{\,n}}{\Delta t} = \frac{\theta}{\psi^{n+1}\Delta t}\int_{(\check{X}, t^n)}^{(X, t^{n+1})}\left[\left|X - \hat{X}\right|^2 + (t - t^n)^2\right]^{1/2}\frac{\partial^2 c}{\partial \tau^2}\, d\tau. \tag{4.22}$$

Multiplying both sides by ψ^{n+1} and estimating it in m-norm, we have

$$\left\|\psi^{n+1}\frac{\partial c^{n+1}}{\partial \tau} - \theta\frac{c^{n+1} - \check{c}^{\,n}}{\Delta t}\right\|_m^2 \le \int_\Omega\left[\frac{\psi^{n+1}}{\Delta t}\right]^2\left|\int_{(\check{X}, t^n)}^{(X, t^{n+1})}\frac{\partial^2 c}{\partial \tau^2}\, d\tau\right|^2 dX$$
$$\le \Delta t\left\|\frac{(\psi^{n+1})^3}{\theta}\right\|_\infty\int_\Omega\int_{(\check{X}, t^n)}^{(X, t^{n+1})}\left|\frac{\partial^2 c}{\partial \tau^2}\right|^2 d\tau\, dX$$
$$\le \Delta t\left\|\frac{(\psi^{n+1})^4}{\theta^2}\right\|_\infty\int_\Omega\int_{t^n}^{t^{n+1}}\int_0^1\left|\frac{\partial^2 c}{\partial \tau^2}(\bar{\tau}\check{X} + (1 - \bar{\tau})X,\, t)\right|^2 d\bar{\tau}\, dX dt. \tag{4.23}$$

Therefore, T_4 is bounded by

$$|T_4| \le K\left\|\frac{\partial^2 c}{\partial \tau^2}\right\|_{L^2(t^n,\, t^{n+1};\, m)}^2 \Delta t + K\|\xi^{n+1}\|_m^2. \tag{4.24a}$$

From Lemma 5, T_5 and T_6 are estimated similarly

$$|T_5| \le K\left\{(\Delta t)^{-1}\left\|\frac{\partial \zeta}{\partial t}\right\|_{L^2(t^n,\, t^{n+1};\, m)}^2 + \|\xi^{n+1}\|_m^2\right\}, \tag{4.24b}$$

$$|T_6| \le K\left\{\|\xi^{n+1}\|_m^2 + \|\xi^n\|_m^2 + (\Delta t)^2 + h^4\right\}. \tag{4.24c}$$

$T_7, T_8,$ and T_9 are argued as follows. If f is a function defined on Ω, denoting one of three functions $c, \zeta,$ and $\xi,$ and Z means the unit vector of $\mathbf{U}^{n+1} - \mathbf{u}^{n+1}$, then

$$\int_\Omega \theta \frac{\hat{f}^n - \check{f}^n}{\Delta t} \xi^{n+1} dX$$

$$= (\Delta t)^{-1} \int_\Omega \theta \left[\int_{\check{X}}^{\hat{X}} \frac{\partial f^n}{\partial Z} \right] \xi^{n+1} dX$$

$$= (\Delta t)^{-1} \int_\Omega \theta \left[\int_0^1 \frac{\partial f^n}{\partial Z} ((1 - \overline{Z})\check{X} + \overline{Z}\hat{X}) d\overline{Z} \right] \left| \hat{X} - \check{X} \right| \xi^{n+1} dX$$

$$= \int_\Omega \left[\int_0^1 \frac{\partial f^n}{\partial Z} ((1 - \overline{Z})\check{X} + \overline{Z}\hat{X}) d\overline{Z} \right] |\mathbf{u} - \mathbf{U}| \xi^{n+1} dX, \tag{4.25}$$

where the parameter $\overline{Z} \in [0, 1]$, $\hat{X} - \check{X} = \Delta t[\mathbf{u}^{n+1}(X) - \mathbf{U}^{n+1}(X) / \theta(X)$. Define

$$g_f = \int_0^1 \frac{\partial f^n}{\partial Z} ((1 - \overline{Z})\check{X} + \overline{Z}\hat{X}) d\overline{Z},$$

then we obtain three special inequalities from (4.25),

$$|T_7| \le \|g_c\|_\infty \|(\mathbf{u} - \mathbf{U})^{n+1}\|_m \|\xi^{n+1}\|_m, \tag{4.26a}$$

$$|T_8| \le \|g_\zeta\|_m \|(\mathbf{u} - \mathbf{U})^{n+1}\|_m \|\xi^{n+1}\|_\infty, \tag{4.26b}$$

$$|T_9| \le \|g_\xi\|_m \|(\mathbf{u} - \mathbf{U})^{n+1}\|_m \|\xi^{n+1}\|_\infty. \tag{4.26c}$$

From Lemma 1-Lemma 5, and (4.8), we have

$$\|(\mathbf{u} - \mathbf{U})^{n+1}\|_m^2 \le K \left\{ \|\xi^n\|_m^2 + h_p^4 + h_c^4 + (\Delta t)^2 \right\}. \tag{4.27}$$

Since $g_c(X)$ is the mean value of first-order partial derivatives of c^n, it could be estimated by $\|c^n\|_{W_\infty^1}$. It follows from (4.26a),

$$|T_7| \le K\left\{\|\xi^{n+1}\|_m^2 + \|\xi^n\|_m^2 + h_p^4 + h_c^4 + (\Delta t)^2\right\}. \tag{4.28}$$

In order to estimate $\|g_\zeta\|_m$ and $\|g_\xi\|_m$, we introduce the following induction hypothesis:

$$\sup_{0\le n\le L}\|\sigma\|_\infty \to 0,\ \sup_{0\le n\le L}\|\xi^n\|_m \to 0,\ (h_c,\ h_p,\ \Delta t) \to 0, \tag{4.29}$$

and the partition restriction

$$\Delta t = O(h^2),\ h^2 = o(h_p^{3/2}). \tag{4.30}$$

Considering

$$\|g_f\|^2 \le \int_0^1\int_\Omega\left[\frac{\partial f^n}{\partial Z}((1-\overline{Z})\check{X} + \overline{Z}\hat{X})\right]^2 dXd\overline{Z}. \tag{4.31}$$

Using the transformation,

$$G_{\overline{Z}}(X) = (1-\overline{Z})\check{X} + \overline{Z}\hat{X} = X - [\theta^{-1}(X)\mathbf{u}^{n+1}(X) + \overline{Z}\theta^{-1}(X)(\mathbf{U}-\mathbf{u})^{n+1}(X)]\Delta t, \tag{4.32}$$

then, we have

$$\|g_f\|^2 \le \int_0^1\sum_{J_p}\left|\frac{\partial f^n}{\partial Z}(G_{\overline{Z}}(X))\right|^2 dXd\overline{Z}, \tag{4.33}$$

where $J_p = \Omega_{ijk} = [x_{i-1/2},\ x_{i+1/2}]\times[y_{j-1/2},\ y_{j+1/2}]\times[z_{k-1/2},\ z_{k+1/2}]$ denotes a grid element of the flow equation.

It follows from (4.29) and (4.30),

$$\det DG_{\overline{Z}} = 1 + o(1).$$

Then, Equation (4.33) is estimated by

$$\|g_f\|^2 \le K\|\nabla f^n\|^2. \tag{4.34}$$

Using (4.34), Lemma 5 and the Sobolev embedding theorem [1], we could estimate T_8,

$$\begin{aligned}|T_8| &\le K\,\|\nabla\zeta^n\|\cdot\|(\mathbf{u}-\mathbf{U})^{n+1}\|\cdot h^{-(\varepsilon+1/2)}\|\nabla\xi^{n+1}\|\\ &\le K\left\{h_c^{2-(\varepsilon+1/2)}\|(\mathbf{u}-\mathbf{U})^{n+1}\|\,\|\nabla\xi^{n+1}\|\right\}\\ &\le K\left\{\|\xi^{n+1}\|_m^2+\|\xi^n\|_m^2+h_p^4+h_c^4+(\Delta t)^2\right\}+\varepsilon|\|\alpha^{n+1}\||^2. \end{aligned}\tag{4.35a}$$

From (4.27), we find that $\|(\mathbf{u}-\mathbf{U})^{n+1}\|_m = o(h_c^{-(\varepsilon+1/2)})$. Therefore, it is necessary to prove $\|\xi^n\|_m = O(h_p^2+h_c^2+\Delta t)$. Using the argument similar to [36], we have

$$\begin{aligned}|T_9| &\le K\,\|\nabla\xi^n\|\cdot\|(\mathbf{u}-\mathbf{U})^{n+1}\|\cdot h^{-(\varepsilon+1/2)}\|\nabla\xi^{n+1}\|\\ &\le \varepsilon\left\{|\|\alpha^{n+1}\||^2+|\|\alpha^n\||^2\right\}. \end{aligned}\tag{4.35b}$$

T_{10} and T_{11} are treated by using the negative norm estimates

$$|T_{10}| \le K h_c^4+\varepsilon\,|\|\alpha^{n+1}\||^2, \tag{4.36a}$$

$$|T_{11}| \le K\,\|\xi^n\|_m^2+\varepsilon\,|\|\alpha^{n+1}\||^2. \tag{4.36b}$$

Considering the resulting estimates (4.20), (4.21), (4.24), (4.28), (4.35), (4.36), and (4.19) together, we have

$$\begin{aligned}&\frac{1}{2\Delta t}\{(\theta\xi^{n+1},\,\xi^{n+1})_m-(\theta\xi^n,\,\xi^n)_m\}+\sum_{s=x,y,z}(D^{-1}\alpha^{s,n+1},\,\alpha^{s,n+1})_s\\ &\le K\,\{\left\|\frac{\partial^2 c}{\partial\tau^2}\right\|^2_{L^2(t^n,t^{n+1};m)}\Delta t+(\Delta t)^{-1}\left\|\frac{\partial\zeta}{\partial t}\right\|^2_{L^2(t^n,t^{n+1};m)}+\|\xi^{n+1}\|_m^2+\|\xi^n\|_m^2\\ &\quad+\|\mu^n\|_m^2+h_p^4+h_c^4+(\Delta t)^2\}+\varepsilon\left\{|\|\alpha^{n+1}\||^2+|\|\alpha^n\||^2\right\}. \end{aligned}\tag{4.37}$$

Multiplying (4.37) by $2\Delta t$, summing them on $n(0 \le n \le L)$, and noting that $\xi^0 = 0$, we have

$$\|\xi^{L+1}\|_m^2 + \sum_{n=0}^{L} |||\alpha^{n+1}|||^2 \Delta t \le K \{\sum_{n=0}^{L} \left[\|\xi^{n+1}\|_m^2 + \|\mu^n\|_m^2\right]\Delta t + h_p^4 + h_c^4 + (\Delta t)^2\}. \tag{4.38}$$

It holds for (4.16b) from $\mu^0 = 0$,

$$\|\mu^{L+1}\|_{L^2}^2 \le K \{\sum_{n=1}^{L} \left[\|\mu^n\|_{L^2}^2 + \|\xi^n\|_{L^2}^2\right]\Delta t + h_c^4 + h_p^4 + (\Delta t)^2\}. \tag{4.39}$$

Considering (4.38), (4.39) and the relation of continuous L^2-norm and discrete m-norm [14, 25] together, we obtain

$$\|\xi^{L+1}\|_m^2 + \|\mu^{L+1}\|_{L^2}^2 + \sum_{n=0}^{L} |||\alpha^{n+1}|||^2 \Delta t \le K \{\sum_{n=0}^{L} \left[\|\xi^{n+1}\|_m^2 + \|\mu^n\|_{L^2}^2\right]\Delta t + h_p^4 + h_c^4 + (\Delta t)^2\}. \tag{4.40}$$

Applying the Gronwall lemma, we get

$$\|\xi^{L+1}\|_m^2 + \|\mu^{L+1}\|_{L^2}^2 + \sum_{n=0}^{L} |||\alpha^{n+1}|||^2 \Delta t \le K \{h_p^4 + h_c^4 + (\Delta t)^2\}. \tag{4.41a}$$

By (4.41a), (4.8), and (4.14), we have

$$\sup_{0 \le n \le L} \left\{\|\pi^{n+1}\|_m^2 + |||\alpha^{n+1}|||^2\right\} \le K\{h_p^4 + h_c^4 + (\Delta t)^2\}. \tag{4.41b}$$

It remains to testify the induction hypothesis (4.29). For $n = 0$, it is true obviously by using the initial conditions and $\xi^0 = 0$. Suppose that it holds for $1 \le n \le L$. Then, it follows from (4.41) and (4.30),

$$|||\sigma^{L+1}|||_\infty \le K h_p^{-3/2} \{h_p^2 + h_c^2 + \Delta t\} \le K h_p^{1/2} \to 0, \tag{4.42a}$$

$$\|\xi^{L+1}\|_\infty \le Kh_c^{-3/2}\{h_p^2 + h_c^2 + \Delta t\} \le Kh_c^{1/2} \to 0. \tag{4.42b}$$

Therefore, it holds for $n = L + 1$ and the proof is completed.

The following theorem is concluded from (4.41), Lemma 5 and Lemma 6.

Theorem 3. *Suppose that the conditions* (R) *and* (C) *hold. Numerical solutions are obtained by using the procedures* (3.3), (3.4), *and* (3.5). *If the restriction* (4.30) *holds, then*

$$\|p - P\|_{\overline{L}^\infty(J;m)} + \|\mathbf{u} - \mathbf{U}\|_{\overline{L}^\infty(J;V)} + \|c - C\|_{\overline{L}^\infty(J;m)} + \|\mathbf{g} - \mathbf{G}\|_{\overline{L}^2(J;V)}$$

$$+ \|s - S\|_{\overline{L}^\infty(J;L^2)} \le M^*\{h_p^2 + h_c^2 + \Delta t\}, \tag{4.43}$$

where $\|g\|_{\overline{L}^\infty(J;X)} = \sup_{n\Delta t \le T}\|g^n\|_X$, $\|g\|_{\overline{L}^2(J;X)} = \sup_{L\Delta t \le T}\{\sum_{n=0}^{L}\|g^n\|_X^2\Delta t\}^{1/2}$, *and the constant* M^* *depends on p, c, s and their derivatives.*

5. Modified Mixed Volume Element with Characteristic Volume Element and its Numerical Analysis

In Sections 3 and 4, we discuss the method of mixed volume element with characteristic volume element. While in actual applications, Darcy velocity changes more slow than the concentration with respect to t. Therefore, a large time step may be used for solving Equation (1.1). The interval J is partitioned by $0 = t_0 < t_1 < \cdots < t_L = T$. Let $\Delta t_p^m = t_m - t_{m-1}$, and suppose that the partition is measured uniformly by $\Delta t_p^m = \Delta t_p$, $m \ge 2$ except Δt_p^1. The concentration is computed by a small uniform step $\Delta t_c = t^n - t^{n-1}$. Suppose that there exists a positive integer n corresponding to m such that the pressure and the concentration have the same nodes, $t_m = t^n$. Let $j = \Delta t_p / \Delta t_c$ and $j_1 = \Delta t_p^1 / \Delta t_c$. Let

$\psi_m(X) = \psi(X, t_m)$. Darcy velocity $\mathbf{u}^{n+1}$ at t^{n+1}, $t_{m-1} < t^{n+1} \le t_m$, in (3.4) is defined as follows. The approximation is defined by a linear extrapolation of $\mathbf{U}_{m-1}$ and $\mathbf{U}_{m-2}$ for $m \ge 2$,

$$E\mathbf{U}^{n+1} = (1 + \frac{t^{n+1} - t_{m-1}}{t_{m-1} - t_{m-2}})\mathbf{U}_{m-1} - \frac{t^{n+1} - t_{m-1}}{t_{m-1} - t_{m-2}}\mathbf{U}_{m-2}. \tag{5.1}$$

If $m = 1$, define $E\mathbf{U}^{n+1} = \mathbf{U}_0$.

The procedures of (1.1) and (1.2) are formulated. Numerical solutions $(\mathbf{U}_m, P_m): (t_0, t_1, \cdots, t_L) \to S_h \times V_h$ and $(C^n, \mathbf{G}^n, C'^n): (t^0, t^1, \cdots, t^R) \to S_h \times V_h \times M_h$ are computed by

$$(D_x U_m^x + D_y U_m^y + D_z U_m^z, v)_{\hat{m}} = (q_m, v)_{\hat{m}}, \ \forall v \in S_h, \tag{5.2a}$$

$$(k^{-1}(\overline{C}_m^x)U_m^x, w^x)_x + (k^{-1}(\overline{C}_m^y)U_m^y, w^y)_y + (k^{-1}(\overline{C}_m^z)U_m^z, w^z)_z$$

$$- (P_m, D_x w^x + D_y w^y + D_z w^z)_{\hat{m}} = 0, \ \forall \mathbf{w} \in V_h. \tag{5.2b}$$

For clarity, the previous m-norm is replaced by $\hat{m}$-norm.

$$\left(\theta \frac{C^{n+1} - \hat{C}^n}{\Delta t}, v\right)_{\hat{m}} + \left(\rho \frac{C'^{n+1} - C'^n}{\Delta t}, v\right)_{\hat{m}} + (D_x G^{x,n+1} + D_y G^{y,n+1}$$

$$+ D_z G^{z,n+1}, v)_{\hat{m}} = \left(f(\hat{C}^n), v\right)_{\hat{m}}, \ \forall v \in S_h, \tag{5.3a}$$

$$(D^{-1}G^{x,n+1}, w^x)_x + (D^{-1}G^{y,n+1}, w^y)_y + (D^{-1}G^{z,n+1}, w^z)_z - (C^{n+1}, D_x w^x$$

$$+ D_y w^y + D_z w^z)_{\hat{m}} = 0, \ \forall \mathbf{w} \in V_h, \tag{5.3b}$$

$$\left(\frac{S^{n+1} - S^n}{\Delta t}, \varphi\right)_{L^2} = \hat{\alpha}(\phi(C^n) - S^n, \varphi)_{L^2}, \quad \forall \varphi \in M_h, \tag{5.4}$$

where $\hat{C}^n = C^n(X - \theta^{-1}E\mathbf{U}^{n+1}\Delta t)$.

$$C^0 = \widetilde{C}^0, \quad G^0 = \widetilde{G}^0, \quad S^0 = \widetilde{S}^0, \quad X \in \Omega. \tag{5.5}$$

The procedures (5.2), (5.3), (5.4), and (5.5) are carried out similarly to (3.3)-(3.6) of Section 3. Here it is pointed out that Equations (1.1) and (1.2) are discretized with two different steps. It can shorten the computational work greatly without losing accuracy.

In a similar analysis to Theorem 3, we conclude the following result.

Theorem 4. *Suppose that exact solutions of* (1.1)-(1.7) *are regular* (R), *and the coefficients are positive definite* (C). *Adopting the procedures* (5.2)-(5.5) *to obtain numerical solutions*, *under the restriction* (4.30), *we have*

$$\|p - P\|_{\bar{L}^\infty(J;m)} + \|\mathbf{u} - \mathbf{U}\|_{\bar{L}^\infty(J;V)} + \|c - C\|_{\bar{L}^\infty(J;m)} + \|\mathbf{g} - \mathbf{G}\|_{\bar{L}^2(J;V)}$$

$$+ \|s - S\|_{\bar{L}^\infty(J;L^2)} \le M^{**}\left\{h_p^2 + h_c^2 + \Delta t_c + (\Delta t_p)^2 + (\Delta t_p^1)^{3/2}\right\}, \qquad (5.6)$$

where the constant M^{**} *depends on p, c, s and their derivatives.*

6. Numerical Experiment

Consider a one-dimensional problem on $\Omega = [0, 1]$,

$$\frac{\partial c}{\partial t} + (\phi(c))_t + \mathbf{u} \cdot \nabla c - D\Delta c = 0. \qquad (6.1)$$

We use the method of mixed volume element with characteristic mixed volume element to solve Equation (6.1) with the following assumptions:

(1) $u = 1$, $D = 0.01$; (2) $\phi(c) = e^p$; (3) the initial value = 0; (4) the value at the left-hand endpoint = 1, the value at the right-hand endpoint = 0.

Numerical solutions at $t = 0.5$ are illustrated for $p = 0.5$ and $p = 1$ in Figures 2 and 3 respectively.

The change of the concentration c as $p = 0.5$ is shown in Figure 2. From Figure 3, we see that the curve of c is more smooth as $p = 1$ comparison with Figure 2. Then, we conclude that the value of p is effective in computing the concentration.

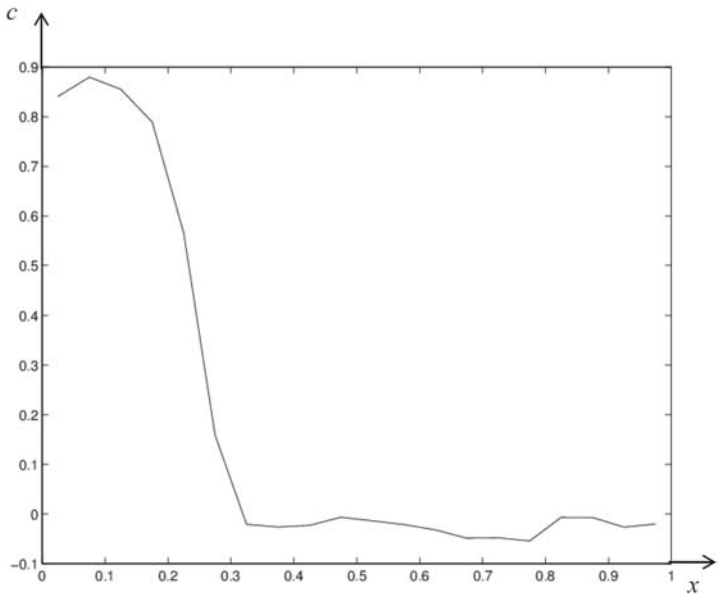

Figure 2. Numerical illustration of $p = 0.5$.

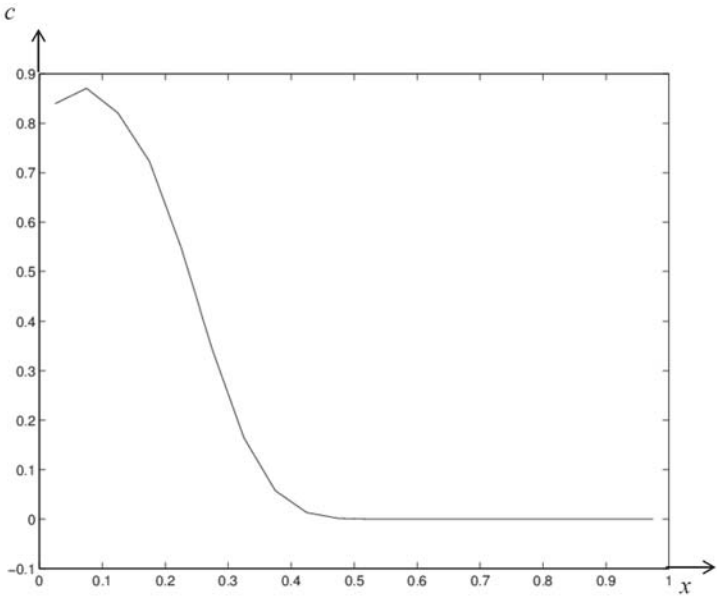

Figure 3. Numerical illustration of $p = 1$.

Next, we consider a two-dimensional convection-diffusion equation and solve it by using the characteristic mixed volume element

$$\begin{cases} \dfrac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c - \nabla(D\nabla c) = f, & X \in \Omega,\ 0 < t \le T, \\ c(X,\ 0) = c_0, & X \in \Omega, \\ \dfrac{\partial c}{\partial \nu} = 0, & X \in \partial\Omega,\ 0 < t \le T, \end{cases} \tag{6.2}$$

where $\Omega = (0,\ 1) \times (0,\ 1)$ and ν denotes the outer unit vector to $\partial\Omega$. Define $\mathbf{u} = (u_1,\ u_2)^T$ and $D(x,\ y)$ as

$$u_1 = 1 + x^2,$$

$$u_2 = 1 + y^2,$$

$$D(x,\ y) = 10^{-4} + xy.$$

The right-hand side function f is chosen properly such that exact solution is defined by

$$c = e^{-\pi^2 t} \cos(2\pi x) \cos(2\pi y).$$

Obviously, $c_0(x,\ y) = \cos(2\pi x) \cos(2\pi y)$.

Here we use the presented method to solve (6.2), and evaluate the function c and its gradient $g = \nabla c$. Take $T = 0.03$, $h = 1 / N$, $\Delta t = 4h^2$. Numerical data of $c(x,\ y,\ t)$ and $g(x,\ y,\ t)$ are shown in Tables 1 and 2 respectively. Let $\|r\|^2 = \sum_{i,\ j=1}^{N} r_{ij}^2 h^2$, $\|\nabla r\|^2 = \sum_{i=1}^{N}$, and let C and G denote the numerical solutions. Table 1 shows error estimates of center finite difference (CFD), the method of characteristics (MOC), and characteristic mixed volume element (CMVE) on different meshes.

Table 1. Error estimates of $\|c - C\| * 10^4$

N	CFD	MOC	CMVE
40	45.706668	41.627797	33.751945
80	12.392356	10.866577	8.627756
120	5.667990	4.878326	3.965134
160	3.228423	2.745332	2.342464
200	2.073806	1.750132	1.609548
240	1.439614	1.234541	1.209797

Table 2. Error estimates of $\|g - G\| * 10^3$ by the CMVE

N	CMVE	N	CMVE
40	17.155501	160	4.493999
80	8.854135	200	3.608725
120	5.960560	240	3.017028

From Tables 1 and 2, we find that the CMVE could solve c and g simultaneously and efficiently comparison with CFD and MOC.

7. Conclusions and Discussions

Numerical approximation and theoretical analysis of three-dimensional contamination transport are considered in this paper. A type of mixed volume element-characteristic mixed volume element method is discussed. Several interesting conclusions are stated as follows.

(I) The method has the physical nature of conservation (local and whole), an important physical nature in numerical simulation of underground environmental science problems.

(II) The composite method combines a mixed volume element and the idea of characteristics, so it has strong stability and high accuracy. It is quite useful especially in large-scaled engineering computation on a three-dimensional complicated region.

(III) The method develops the convergence result of $3/2$-order of Arbogast and Wheeler to second order, and possibly solves the problems better [2, 17, 28, 31].

In the following research, the authors would pay more attention to the topics. (1) Combining the recent work [37-43], the authors try to study the physical equations and put forward new numerical methods. (2) Using actual data of (1.1)-(1.7), the authors try to accomplish numerical tests and give a professional software for environmental treatment. (3) Studying the recent research on variational formulation and fractal calculus, this work may possibly be continued for the contamination transport [44-52].

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