

# The Theory and Application of Upwind Finite Difference Fractional Steps Procedure for Seawater Intrusion

Yirang Yuan, Hongxing Rui, Dong Liang, Changfeng Li

Institute of Mathematics, Shandong University, Jinan, China

Email: yryuan@sdu.edu.cn

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## ABSTRACT

Numerical simulation and theoretical analysis of seawater intrusion is the mathematical basis for modern environmental science. Its mathematical model is the nonlinear coupled system of partial differential equations with initial-boundary problems. For a generic case of a three-dimensional bounded region, two kinds of finite difference fractional steps procedures are put forward. Optimal order estimates in  $l^2$  norm are derived for the error in the approximation solution. The present method has been successfully used in predicting the consequences of seawater intrusion and protection projects.

**Keywords:** Seawater Intrusion; Three-Dimensional Region; Upwind Fractional Steps;  $l^2$  Norm Estimate; Numerical Simulation

## 1. Introduction

Seawater intrusion refers to the invasion of salt water into the groundwater in coastal areas caused by the changes in natural water environment and social and economic development. In recent years, it has occurred in many countries in the world such as USA, Netherlands, Israel and Japan. After 1970s, the northern coastal area of our country, especially economic zones around Bohai such as Shandong, Hebei and Liaoning, is getting more and more seriously affected by this problem with Shandong province standing out. It leads to the great decrease in industrial and agricultural production, making people's living conditions, especially their drinking water, poorer and poorer. Therefore, it is urgent that seawater intrusion be completely tackled.

The mathematical model consists of water head equation and salt concentration equation. Because of the compressibility of porous media and that of the fluid, the change in fluid density with the salt concentration, and with the consideration of the fact that the salt is in the moving state in porous media, there may occur convection-dominated diffusion. While water is moving in the water-bearing stratum, it carries salt. The movement of this solute with underground water is called solute convection. Since salt is inhomogeneously distributed in the whole solution, it always diffuses from places with higher concentration to places with lower concentration even if the solution does not move.

### 1.1. Water Head Equation

With Darcy's law, Euler method and Huyakorn's linearization method, the water head equation is obtained [1,2].

$$S_s \frac{\partial H}{\partial t} - \nabla \cdot (K(\nabla H - \eta c e_3)) = -\psi \eta \frac{\partial c}{\partial t} + \frac{\rho}{\rho_0} q, (x, y, z)^T \in \Omega, t \in J = (0, T], \quad (1)$$

where  $S_s$  is the specific retention,  $H = p/(\rho_0 g) - z$  is water head function,  $p$  stands for pressure,  $\rho_0$  represents the density of reference water (fresh water),  $g$  is gravitational acceleration,  $z$  is the height of water containing layer,  $\rho$  is density and depends only on the concentration of salt  $c$ , Hugakorn's linearization  $\rho = \rho_0(1 + \varepsilon c/c_s)$  is adopted.  $c_s$  is the concentration corresponding to the maximum density, and  $\varepsilon$  is the density difference ration  $\varepsilon = (\rho_s - \rho_0)/\rho_0$ .  $K = K\rho g/\mu$ ,  $\mu$  is viscosity of the fluid,  $\eta = \varepsilon/c_s$  is the density coupling coefficient.  $e_3 = (0, 0, 1)^T$ ,  $\psi$  is the porosity,  $q$  is source or sink term, and the permeability is noted by

$$K = \begin{bmatrix} K_1 & 0 & 0 \\ 0 & K_2 & 0 \\ 0 & 0 & K_3 \end{bmatrix}$$

### 1.2. Salt Concentration Equation

The movement of  $Cl^-$  dissolved in the fluid causes

convection and diffusion of  $Cl^-$  in porous media. From Fick's law and mass conservation law we have the following concentration Equation [1,2].

$$\begin{aligned} \psi \frac{\rho_0}{\rho} \frac{\partial c}{\partial t} &= \nabla \cdot (\psi D \nabla c) - \mathbf{u} \cdot \nabla c \\ &+ q(C^* - c), (x, y, z)^T \in \Omega, t \in J, \end{aligned} \tag{2}$$

where  $c$  stands for the concentration of  $Cl^-$ ,  $C^*$  is the salt concentration near the source well. Darcy's velocity and the diffusion matrix are denoted by

$$\mathbf{u} = -\frac{\rho_0}{\rho} K (\nabla H - \eta c \mathbf{e}_3)$$

and

$$D = \begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix}.$$

### 1.3. Initial Boundary Value Conditions

To make a complete system, appropriate initial boundary value conditions are necessary in addition to the above equations. The initial value condition is

$$\begin{aligned} H(x, y, z, 0) &= H_0(x, y, z), c(x, y, z, 0) \\ &= c_0(x, y, z), (x, y, z) \in \Omega. \end{aligned} \tag{3}$$

There are three kinds of boundary value conditions. When concentration and water head are known, the first kind of boundary value condition can be given as

$$\begin{aligned} H(x, y, z, t) &= h(x, y, z, t), c(x, y, z, t) \\ &= g(x, y, z, t), (x, y, z) \in \Gamma_1, t \in J. \end{aligned} \tag{4a}$$

The second kind of boundary value condition can be given to non-flow boundary:

$$\mathbf{u} \cdot \mathbf{n} = 0, D \nabla c \cdot \mathbf{n} = 0, (x, y, z) \in \Gamma_2, t \in J \tag{4b}$$

where  $\mathbf{n}$  is the unit vector in outer normal direction. A kind of Stefan boundary condition is for free surface boundary.

The boundary condition of water heat equation:

$$\begin{aligned} H &= -z, (x, y, z) \in \Gamma_3 \\ \frac{\partial H}{\partial t} + \frac{1}{\mu} (\mathbf{u} - \mathbf{w}) \cdot \nabla (H + z) &= 0, (x, y, z) \in \Gamma_3, t \in J. \end{aligned} \tag{4c}$$

The boundary condition of salt concentration equation:

$$\begin{aligned} \psi D \nabla c \cdot \mathbf{n} &= (1 - \mu_0) (\mathbf{u} - \mathbf{w}) \cdot \mathbf{n} (c - c'), \\ (x, y, z) &\in \Gamma_3, t \in J. \end{aligned}$$

where  $\mathbf{w}$  is the permeated fluid flow rate in a unit area and  $c'$  is the concentration of  $Cl^-$  in permeated fluid.

In the study of seawater intrusion miscible model, for

the miscible fluid Henry suggested an analytic solution under the simplified boundary condition and with the steady-state flow in the homogeneous medium [3]. Segol, Pinder, Grug, Heinrich and others studied the two-dimensional cut plane problem [4,5], and Huyakorn, Gupta and Yapa studied the solving process of the three-dimensional problem [5,6]. However, their calculations are made in specifically assumed conditions; therefore, they can not truly reflect seawater intrusion.

For plane incompressible two-phase displacement which is assumed to be  $\Omega$ -periodic, Jim Douglas, Ewing, Russell, and others have published famous papers on the characteristic finite difference method and finite element method to solve the convection-dominated diffusion problems with finite difference method, and to overcome oscillation and faults likely to occur in the traditional methods [7-12]. For compressible two-phase displacement problem, Douglas and others have contributed much to the mathematical model of "infinitesimal compressibility", numerical method and analysis [13-16]. Douglas and Yuan discarded periodic conditions, put forward a new modified characteristic finite difference method and finite element method, and obtained optimal order estimation in  $l^2$  norm [17-20]. Special treatment is needed for characteristic lines because the method of characteristics asks for interpolation and they may go through the boundaries near the solution regions. It is necessary to find out the intersection point of characteristic lines and mesh boundaries and calculate their corresponding functional values. While such calculation is designed, we must determine whether characteristic lines really go through the boundaries in order to decide whether time steps lengths should be changed. In a word, the practical calculation is quite complicated [19,20].

For the convection-dominated diffusion problems, Axelsson, Ewing, Lazarov and others proposed upwind finite difference method [21-23] to overcome oscillation and to avoid computation complexity of the characteristic differential method near boundary meshes. Douglas and Peaceman applied the alternating-direction method to numerical reservoir simulation [24,25]. By using Fourier analysis, they succeeded in proving the stability and convergence according to the constant coefficient [26,27]. This paper, starting from the actual case, puts forward the modified method of upwind with finite difference fractional steps procedure for seawater intrusion. It can overcome oscillation and diffusion and computational complexity. At the same time it can convert a three-dimensional problem into three successive one-dimensional problems, reducing computation complexity and making computation practical. Moreover, it increases the space calculation accuracy to the second order. Some techniques, such as calculus of variations, energy method, operator-splitting, upwind method, commutative law of

multiplication of difference operators, decomposition of high order difference operators, the theory of prior estimates and techniques are adopted. Optimal order estimates in  $L^2$  norm are derived to determine the error in the approximate solution. Thus the difficult problem has been solved [16,28].

Generally, this is a positive definite problem:

$$0 < K_* \leq K_i(c) \leq K^*, \left| \partial^2 K_i(c) / \partial t^2 \right| \leq K^*, i = 1, 2, 3, \tag{5}$$

$$0 < D_* \leq D(x, y, z, t) \leq D^*, 0 < \Psi_* \leq \Psi(x, y, z) \leq \Psi^*,$$

where  $K_*$ ,  $K^*$ ,  $\Psi_*$ ,  $\Psi^*$  are constants.

Our assumptions on the regularity of the solution of (1)-(5) are denoted collectively by

$$H, c \in L^\infty(W^{4,\infty}) \cap W^{1,\infty}(W^{1,\infty}),$$

$$\partial^2 H / \partial t^2, \partial^2 c / \partial t^2 \in L^\infty(L^\infty).$$

In this paper  $M$  and  $\varepsilon$  express general positive constant and general positive small constant respectively, and have different meanings.

$$\delta_{\bar{x}} \left( K(C_h^n) \delta_x H_h^{n+1} \right)_{ijk} = h_1^{-2} \left[ K(C_h^n)_{i+1/2,jk} \left( H_{h,i+1,jk}^{n+1} - H_{h,ijk}^{n+1} \right) - \left( H_{h,ijk}^{n+1} - H_{h,i-1,jk}^{n+1} \right) \right], \tag{6a}$$

$$\delta_{\bar{y}} \left( K(C_h^n) \delta_y H_h^{n+1} \right)_{ijk} = h_2^{-2} \left[ K(C_h^n)_{i,j+1/2,k} \left( H_{h,i,j+1,k}^{n+1} - H_{h,ijk}^{n+1} \right) - \left( H_{h,ijk}^{n+1} - H_{h,i,j-1,k}^{n+1} \right) \right], \tag{6b}$$

$$\delta_{\bar{z}} \left( K(C_h^n) \delta_z H_h^{n+1} \right)_{ijk} = h_3^{-2} \left[ K(C_h^n)_{ij,k+1/2} \left( H_{h,ij,k+1}^{n+1} - H_{h,ijk}^{n+1} \right) - \left( H_{h,ijk}^{n+1} - H_{h,ij,k-1}^{n+1} \right) \right], \tag{6c}$$

$$\nabla_h \left( K(C_h^n) \nabla H_h^{n+1} \right)_{ijk} = \delta_{\bar{x}} \left( K(C_h^n) \delta_x H_h^{n+1} \right)_{ijk} + \delta_{\bar{y}} \left( K(C_h^n) \delta_y H_h^{n+1} \right)_{ijk} + \delta_{\bar{z}} \left( K(C_h^n) \delta_z H_h^{n+1} \right)_{ijk}. \tag{7}$$

Let  $H_{h,ijk}^n$  and  $C_{h,ijk}^n$  be the finite difference solutions of  $H(X_{ijk}, t^n)$  and  $c(X_{ijk}, t^n)$ , respectively. If the finite difference solutions  $C_h^n$  and  $H_h^n$  are known, we find the finite difference solutions  $C_h^{n+1}$ ,  $H_h^{n+1}$  at  $t^{n+1}$ .

## 2. The Upwind Finite Difference Fractional Steps Procedure

For brevity we consider only the first kind of boundary value problem and the diffusion matrix  $D(x, y, z)$  of diagonal form. In order to get the solution by using finite difference method we use mesh region  $\Omega_h$  instead of region  $\Omega$ . On space  $(x, y, z)$ , let step lengths be  $h_3$ ,  $x_i = ih_1$ ,  $y_j = jh_2$ ,  $z_k = kh_3$ ,

$$\Omega_h = \left\{ (x_i, y_j, z_k) \left| \begin{array}{l} i_1(j, k) < i < i_2(j, k) \\ j_1(i, k) < j < j_2(i, k) \\ k_1(i, j) < k < k_2(i, j) \end{array} \right. \right\}.$$

Let  $\partial\Omega_h$  stands for the boundaries of  $\Omega_h$ ,  $X_{ijk} = (ih_1, jh_2, kh_3)^T$ ,  $t^n = n\Delta t$ ,  $W(X_{ijk}, t^n) = W_{ijk}^n$ . Let

$$K(C_h^n)_{i+1/2,jk} = \left[ K(X_{ijk}, C_{h,ijk}^n) + K(X_{i+1,jk}, C_{h,i+1,jk}^n) \right] / 2,$$

$$K(C_h^n)_{i,j+1/2,k} = \left[ K(X_{ijk}, C_{h,ijk}^n) + K(X_{i,j+1,k}, C_{h,i,j+1,k}^n) \right] / 2,$$

$$K(C_h^n)_{ij,k+1/2} = \left[ K(X_{ijk}, C_{h,ijk}^n) + K(X_{ij,k+1}, C_{h,ij,k+1}^n) \right] / 2,$$

### 2.1. The Second Order Upwind Finite Difference Fractional Steps Scheme

First, compute the approximate Darcy's velocity  $U^n = (U_1^n, U_2^n, U_3^n)^T$  as follows:

$$U_1^n = -\frac{\rho_0}{2} \left\{ \left[ \frac{K_1(C_h^n)}{\rho(C_h^n)} \right]_{i+1/2,jk} \frac{H_{h,i+1,jk}^n - H_{h,ijk}^n}{h_1} + \left[ \frac{K_1(C_h^n)}{\rho(C_h^n)} \right]_{i-1/2,jk} \frac{H_{h,ijk}^n - H_{h,i-1,jk}^n}{h_1} \right\},$$

$$U_2^n = -\frac{\rho_0}{2} \left\{ \left[ \frac{K_2(C_h^n)}{\rho(C_h^n)} \right]_{i,j+1/2,k} \frac{H_{h,i,j+1,k}^n - H_{h,ijk}^n}{h_2} + \left[ \frac{K_2(C_h^n)}{\rho(C_h^n)} \right]_{i,j-1/2,k} \frac{H_{h,ijk}^n - H_{h,i,j-1,k}^n}{h_2} \right\},$$

$$U_3^n = -\frac{\rho_0}{2} \left\{ \left[ \frac{K_3(C_h^n)}{\rho(C_h^n)} \right]_{ij,k+1/2} \frac{H_{h,ij,k+1}^n - H_{h,ijk}^n}{h_3} + \left[ \frac{K_3(C_h^n)}{\rho(C_h^n)} \right]_{ij,k-1/2} \frac{H_{h,ijk}^n - H_{h,ij,k-1}^n}{h_3} \right\}.$$

For salt concentration Equation (2), the modified method of upwind with finite difference fractional steps

scheme is given by

$$\begin{aligned} & \beta(C_{h,ijk}^n) \frac{C_{h,ijk}^{n+1/3} - C_{h,ijk}^n}{\Delta t} \\ &= \left(1 + \frac{h_1}{2} |U_1^n| \bar{D}_1^{-1}\right)^{-1} \delta_x(\bar{D}_1 \delta_x C_h^{n+1/3})_{ijk} \\ &+ \left(1 + \frac{h_2}{2} |U_2^n| \bar{D}_2^{-1}\right)^{-1} \delta_y(\bar{D}_2 \delta_y C_h^n)_{ijk} \\ &+ \left(1 + \frac{h_3}{2} |U_3^n| \bar{D}_3^{-1}\right)^{-1} \delta_z(\bar{D}_3 \delta_z C_h^n)_{ijk} \\ &- \delta_{U_1^n, x} C_{h,ijk}^n - \delta_{U_2^n, y} C_{h,ijk}^n - \delta_{U_3^n, z} C_{h,ijk}^n \\ &+ q_{ijk}^n (C_{h,ijk}^{*,n} - C_{h,ijk}^n), i_1(j, k) < i < i_2(j, k), \\ &C_{h,ijk}^{n+1/3} = g_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h, \end{aligned} \tag{8a}$$

$$\tag{8b}$$

where  $\beta(C) = \psi\rho_0/\rho$ ,  $\bar{D}_i = \psi D_i, i = 1, 2, 3$ .

$$\begin{aligned} & \beta(C_{h,ijk}^n) \frac{C_{h,ijk}^{n+2/3} - C_{h,ijk}^{n+1/3}}{\Delta t} \\ &= \left(1 + \frac{h_2}{2} |U_2^n| \bar{D}_2^{-1}\right)^{-1} \delta_y(\bar{D}_2 \delta_y (C_h^{n+2/3} - C_h^n))_{ijk}, \tag{9a} \\ & j_1(i, k) < j < j_2(i, k), \end{aligned}$$

$$C_{h,ijk}^{n+2/3} = g_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h, \tag{9b}$$

$$\begin{aligned} & \beta(C_{h,ijk}^n) \frac{C_{h,ijk}^{n+1} - C_{h,ijk}^{n+2/3}}{\Delta t} \\ &= \left(1 + \frac{h_3}{2} |U_3^n| \bar{D}_3^{-1}\right)^{-1} \delta_z(\bar{D}_3 \delta_z (C_h^{n+1} - C_h^n))_{ijk}, \tag{10a} \end{aligned}$$

$$k_1(i, j) < k < k_2(i, j), \tag{10b}$$

$$C_{h,ijk}^{n+1} = g_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h,$$

where

$$\delta_{U_1^n, x} c_{ijk} = U_{1,ijk}^n \left[ \bar{H}(U_{1,ijk}^n) \bar{D}_{1,ijk}^{-1} \cdot \bar{D}_{1,i-1/2,jk} \delta_x + (1 - \bar{H}(U_{1,ijk}^n)) \bar{D}_{1,ijk}^{-1} \cdot \bar{D}_{1,i+1/2,jk} \delta_x \right] c_{ijk},$$

$$\delta_{U_2^n, y} c_{ijk} = U_{2,ijk}^n \left[ \bar{H}(U_{2,ijk}^n) \bar{D}_{2,ijk}^{-1} \cdot \bar{D}_{2,i,j-1/2,k} \delta_y + (1 - \bar{H}(U_{2,ijk}^n)) \bar{D}_{2,ijk}^{-1} \cdot \bar{D}_{2,i,j+1/2,k} \delta_y \right] c_{ijk},$$

$$\delta_{U_3^n, z} c_{ijk} = U_{3,ijk}^n \left[ \bar{H}(U_{3,ijk}^n) \bar{D}_{3,ijk}^{-1} \cdot \bar{D}_{3,ij,k-1/2} \delta_z + (1 - \bar{H}(U_{3,ijk}^n)) \bar{D}_{3,ijk}^{-1} \cdot \bar{D}_{3,ij,k+1/2} \delta_z \right] c_{ijk},$$

and  $\bar{H}(z) = \begin{cases} 1, z \geq 0, \\ 0, z < 0. \end{cases}$

Next, for fluid Equation (1) the fractional steps sinite difference scheme is given by

$$\begin{aligned} & S_{s,ijk} \frac{H_{h,ijk}^{n+1/3} - H_{h,ijk}^n}{\Delta t} = \delta_x(K_1(C_h^n) \delta_x H_h^{n+1/3})_{ijk} \\ &+ \delta_y(K_2(C_h^n) \delta_y H_h^n)_{ijk} + \delta_z(K_3(C_h^n) \delta_z H_h^n)_{ijk} \\ &- \eta \psi_{ijk} \frac{C_{h,ijk}^{n+1} - C_{h,ijk}^n}{\Delta t} + \frac{\rho(C_{h,ijk}^n)}{\rho_0} q_{ijk}^n \\ &+ \eta \delta_z(K_3(C_h^n) C_h^n)_{ijk}, i_1(j, k) < i < i_2(j, k), \end{aligned} \tag{11a}$$

$$H_{h,ijk}^{n+1/3} = h_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h, \tag{11b}$$

$$\begin{aligned} & S_{s,ijk} \frac{H_{h,ijk}^{n+2/3} - H_{h,ijk}^{n+1/3}}{\Delta t} \\ &= \delta_y(K_2(C_h^n) \delta_y (H_h^{n+2/3} - H_h^n))_{ijk}, \tag{12a} \end{aligned}$$

$$j_1(i, k) < j < j_2(i, k), \tag{12b}$$

$$H_{h,ijk}^{n+2/3} = h_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h,$$

$$\begin{aligned} & S_{s,ijk} \frac{H_{h,ijk}^{n+1} - H_{h,ijk}^{n+2/3}}{\Delta t} \\ &= \delta_z(K_3(C_h^n) \delta_z (H_h^{n+1} - H_h^n))_{ijk}, \tag{13a} \end{aligned}$$

$$k_1(i, j) < k < k_2(i, j), \tag{13b}$$

$$H_{h,ijk}^{n+1} = h_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h.$$

The initial approximation reads

$$C_{h,ijk}^0 = c_0(X_{ijk}), H_{h,ijk}^0 = H_0(X_{ijk}), X_{ijk} \in \Omega_h. \tag{14}$$

The algorithm for a time step is as follows: Assuming the Approximate solution  $\{C_{h,ijk}^n, H_{h,ijk}^n\}$  at time  $t^n$  is known, it is needed to find out the approximate solutions at the next time level. First, compute Darcy's velocity  $\bar{U}^n$ , from schemes (8a), (8b), and method of speedup is used to get the solution of transition sheaf  $\{C_{h,ijk}^{n+1/3}\}$  along  $x$  direction. Secondly, from schemes (9a), (9b) we obtain the solution of transition sheaf  $\{C_{h,ijk}^{n+2/3}\}$ . Thirdly, from schemes (10a), (10b) we obtain solution  $\{C_{h,ijk}^{n+1}\}$ . Next, from (11a), (11b), by using method of speedup, we get the solution of transition sheaf  $\{H_{h,ijk}^{n+1/3}\}$  along  $x$  direction; from (12a), (12b) we obtain the solution of transition sheaf  $\{H_{h,ijk}^{n+2/3}\}$ . Finally, from schemes (13a), (13b) we obtain solution  $\{H_{h,ijk}^{n+1}\}$ . So a complete time

step can be taken. At last, it is because of the positive condition that this finite difference solution exists, being the sole one.

### 2.2. The First Order Weighted Upwind Finite Difference Fractional Steps Scheme

For salt concentration Equation (2), the first order upwind finite difference fractional steps scheme is given by

$$\beta(C_{h,ijk}^n) \frac{C_{h,ijk}^{n+1/3} - C_{h,ijk}^n}{\Delta t} = \delta_x^-(\bar{D}_1 \delta_x C_h^{n+1/3})_{ijk} + \delta_y^-(\bar{D}_2 \delta_y C_h^n)_{ijk} + \delta_z^-(\bar{D}_3 \delta_z C_h^n)_{ijk} - \bar{\delta}_{U_1^n, x} C_{h,ijk}^n - \bar{\delta}_{U_2^n, y} C_{h,ijk}^n - \bar{\delta}_{U_3^n, z} C_{h,ijk}^n + q_{ijk}^n (C_{h,ijk}^{*,n} - C_{h,ijk}^n), i_1(j, k) < i < i_2(j, k), \tag{8a}'$$

$$C_{h,ijk}^{n+1/3} = g_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h, \tag{8b}'$$

$$\beta(C_{h,ijk}^n) \frac{C_{h,ijk}^{n+2/3} - C_{h,ijk}^{n+1/3}}{\Delta t} = \delta_y^-(\bar{D}_2 \delta_y (C_h^{n+2/3} - C_h^n))_{ijk}, j_1(i, k) < j < j_2(i, k), \tag{9a}'$$

$$C_{h,ijk}^{n+2/3} = g_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h, \tag{9b}'$$

$$\beta(C_{h,ijk}^n) \frac{C_{h,ijk}^{n+1} - C_{h,ijk}^{n+2/3}}{\Delta t} = \delta_z^-(\bar{D}_3 \delta_z (C_h^{n+1} - C_h^n))_{ijk}, k_1(i, j) < k < k_2(i, j), \tag{10a}'$$

$$C_{h,ijk}^{n+1} = g_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h, \tag{10b}'$$

where

$$\bar{\delta}_{U_1^n, x} C_{ijk} = \alpha U_{1,ijk}^n \left[ \bar{H}(U_{1,ijk}^n) \delta_x^- + (1 - \bar{H}(U_{1,ijk}^n)) \delta_x^+ \right] C_{ijk} + (1 - \alpha) U_{1,ijk}^n (c_{i+1,j,k} - c_{i-1,j,k}) / 2h_1,$$

and  $\bar{\delta}_{U_2^n, y} C_{ijk}, \bar{\delta}_{U_3^n, z} C_{ijk}$  are defined similarly with a constant  $\alpha \in [0, 1]$ .

The algorithm is similar to that of Scheme (8)-(13).

### 3. Convergence Analysis

For brevity we assume  $\Omega = \{[0, 1]\}^3, h = 1/N, X_{ijk} = (ih, jh, kh)^T, t^n = n\Delta t, W(X_{ijk}, t^n) = W_{ijk}^n$ . Let  $\pi = H - H_h, \xi = c - C_h$ , where  $H$  and  $c$  are the exact solutions of this problem (1) - (5), and  $H_h$  and  $C_h$  are the difference solutions of the schemes (8) - (13).  $\langle \cdot, \cdot \rangle, \|\cdot\|$  and  $\|\cdot\|_1$  denote the inner product and the norms on the discrete spaces  $l^2(\Omega)$  and  $h^1(\Omega)$  corresponding to  $L^2(\Omega)$  and  $H^1(\Omega)$  [19,20,29]. First consider the second order scheme.

**Theorem I.** Suppose that the exact solutions of problem (1)-(5) satisfy condition:

$$H, c \in W^{1,\infty}(W^{1,\infty}) \cap L^\infty(W^{4,\infty}), \partial H / \partial t, \partial c / \partial t \in L^\infty(W^{4,\infty}), \partial^2 H / \partial t^2, \partial^2 c / \partial t^2 \in L^\infty(L^\infty).$$

Adopt the modified method of upwind procedures (8)-(13). Let the dissectible satisfy relation:  $\Delta t = O(h^2)$ . Then the following error estimates hold:

$$\|H - H_h\|_{L^\infty(J;h^1)} + \|c - C_h\|_{L^\infty(J;h^1)} + \|d_t(H - H_h)\|_{L^2(J;h^2)} + \|d_t(c - C_h)\|_{L^2(J;h^2)} \leq M^* (\Delta t + h^2) \tag{15}$$

where  $\|g\|_{L^\infty(J;S)} = \sup_{n\Delta t \leq T} \|g^n\|_S, \|g\|_{L^2(J;S)} = \left( \sum_{n=0}^N \|g^n\|_S^2 \Delta t \right)^{1/2}$ .

Constant  $M^*$  depends on  $H, c$  and their derivatives.

**Proof.** First consider the concentration equation. For Equations (8)-(13), dispel  $C_h^{n+1/3}$  and  $C_h^{n+2/3}$ , and we get the following equivalent form:

$$\beta(C_{h,ijk}^n) \frac{C_{h,ijk}^{n+1} - C_{h,ijk}^n}{\Delta t} - \left\{ \left( 1 + \frac{h}{2} |U_1^n| |\bar{D}_1^{-1}| \right)^{-1} \delta_x^-(\bar{D}_1 \delta_x C_h^{n+1})_{ijk} + \left( 1 + \frac{h}{2} |U_2^n| |\bar{D}_2^{-1}| \right)^{-1} \delta_y^-(\bar{D}_2 \delta_y C_h^{n+1})_{ijk} + \left( 1 + \frac{h}{2} |U_3^n| |\bar{D}_3^{-1}| \right)^{-1} \delta_z^-(\bar{D}_3 \delta_z C_h^{n+1})_{ijk} \right\} = -\delta_{U_1^n, x} C_{h,ijk}^n - \delta_{U_2^n, y} C_{h,ijk}^n - \delta_{U_3^n, z} C_{h,ijk}^n + q_{ijk}^n (C_{h,ijk}^{*,n} - C_{h,ijk}^n) - (\Delta t)^2 \left\{ \left( 1 + \frac{h}{2} |U_1^n| |\bar{D}_1^{-1}| \right)^{-1} \delta_x^-(\bar{D}_1 \delta_x (\beta^{-1}(C_h^n)))_{ijk} \cdot \left( 1 + \frac{h}{2} |U_2^n| |\bar{D}_2^{-1}| \right)^{-1} \delta_y^-(\bar{D}_2 \delta_y d_t C_h^n)_{ijk} + \left( 1 + \frac{h}{2} |U_1^n| |\bar{D}_1^{-1}| \right)^{-1} \delta_x^-(\bar{D}_1 \delta_x (\beta^{-1}(C_h^n)))_{ijk} \cdot \left( 1 + \frac{h}{2} |U_3^n| |\bar{D}_3^{-1}| \right)^{-1} \delta_z^-(\bar{D}_3 \delta_z d_t C_h^n)_{ijk} + \left( 1 + \frac{h}{2} |U_2^n| |\bar{D}_2^{-1}| \right)^{-1} \delta_y^-(\bar{D}_2 \delta_y (\beta^{-1}(C_h^n)))_{ijk} \cdot \left( 1 + \frac{h}{2} |U_3^n| |\bar{D}_3^{-1}| \right)^{-1} \delta_z^-(\bar{D}_3 \delta_z d_t C_h^n)_{ijk} \right\} + (\Delta t)^3 \left( 1 + \frac{h}{2} |U_1^n| |\bar{D}_1^{-1}| \right)^{-1} \delta_x^- \cdot \left( \bar{D}_1 \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |U_2^n| |\bar{D}_2^{-1}| \right)^{-1} \delta_y^-(\bar{D}_2 \delta_y \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |U_3^n| |\bar{D}_3^{-1}| \right)^{-1} \delta_z^-(\bar{D}_3 \delta_z d_t C_h^n) \right) \right) \right)_{ijk}, \tag{16a}$$

$$1 \leq i, j, k \leq N - 1,$$

(16a)

$$C_{h,ijk}^{n+1} = g_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h. \tag{16b}$$

From Equation (2) ( $t = t^{n+1}$ ) and (16) we have the concentration error equations.

$$\begin{aligned} & \beta(C_{h,ijk}^n) \frac{\xi_{h,ijk}^{n+1} - \xi_{h,ijk}^n}{\Delta t} - \left\{ \left( 1 + \frac{h}{2} |U_1^n| \overline{D_1}^{-1} \right)_{ijk}^{-1} \delta_x (\overline{D_1} \delta_x \xi_h^{n+1}) \right. \\ & + \left. \left( 1 + \frac{h}{2} |U_2^n| \overline{D_2}^{-1} \right)_{ijk}^{-1} \delta_y (\overline{D_2} \delta_y \xi_h^{n+1}) + \left( 1 + \frac{h}{2} |U_3^n| \overline{D_3}^{-1} \right)_{ijk}^{-1} \delta_z (\overline{D_3} \delta_z \xi_h^{n+1}) \right\} \\ & = \left[ \delta_{U_1^n, x} C_{h,ijk}^n - \delta_{u_1^{n+1}, x} c_{ijk}^{n+1} \right] + \left[ \delta_{U_2^n, y} C_{h,ijk}^n - \delta_{u_2^{n+1}, y} c_{ijk}^{n+1} \right] + \left[ \delta_{U_3^n, z} C_{h,ijk}^n - \delta_{u_3^{n+1}, z} c_{ijk}^{n+1} \right] \\ & + \left\{ \left[ \left( 1 + \frac{h}{2} |u_1^{n+1}| \overline{D_1}^{-1} \right)_{ijk}^{-1} - \left( 1 + \frac{h}{2} |U_1^n| \overline{D_1}^{-1} \right)_{ijk}^{-1} \right] \delta_x (\overline{D_1} \delta_x C_h^{n+1}) \right. \\ & + \left[ \left( 1 + \frac{h}{2} |u_2^{n+1}| \overline{D_2}^{-1} \right)_{ijk}^{-1} - \left( 1 + \frac{h}{2} |U_2^n| \overline{D_2}^{-1} \right)_{ijk}^{-1} \right] \delta_y (\overline{D_2} \delta_y C_h^{n+1}) \\ & + \left. \left[ \left( 1 + \frac{h}{2} |u_3^{n+1}| \overline{D_3}^{-1} \right)_{ijk}^{-1} - \left( 1 + \frac{h}{2} |U_3^n| \overline{D_3}^{-1} \right)_{ijk}^{-1} \right] \delta_z (\overline{D_3} \delta_z C_h^{n+1}) \right\} \\ & + \left\{ q_{ijk}^{n+1} (C_{h,ijk}^{*,n} - c_{ijk}^{n+1}) - q_{ijk}^n (C_{h,ijk}^{*,n} - C_{h,ijk}^n) \right\} \\ & - (\Delta t)^2 \left[ \left( \left( 1 + \frac{h}{2} |u_1^{n+1}| \overline{D_1}^{-1} \right)_{ijk}^{-1} \delta_x \left( \overline{D_1} \delta_x \left( \beta^{-1}(c^{n+1}) \left( 1 + \frac{h}{2} |u_2^{n+1}| \overline{D_2}^{-1} \right)_{ijk}^{-1} \delta_y (\overline{D_2} \delta_y d_t c^n) \right) \right) \right) \right. \\ & - \left. \left( 1 + \frac{h}{2} |U_1^n| \overline{D_1}^{-1} \right)_{ijk}^{-1} \delta_x \left( \overline{D_1} \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |U_2^n| \overline{D_2}^{-1} \right)_{ijk}^{-1} \delta_y (\overline{D_2} \delta_y d_t C_h^n) \right) \right) \right]_{ijk} \\ & + \left[ \left( 1 + \frac{h}{2} |u_1^{n+1}| \overline{D_1}^{-1} \right)_{ijk}^{-1} \delta_x \left( \overline{D_1} \delta_x \left( \beta^{-1}(c^{n+1}) \left( 1 + \frac{h}{2} |U_2^n| \overline{D_2}^{-1} \right)_{ijk}^{-1} \delta_y (\overline{D_2} \delta_y d_t C_h^n) \right) \right) \right. \\ & - \left. \left( 1 + \frac{h}{2} |U_1^n| \overline{D_1}^{-1} \right)_{ijk}^{-1} \delta_x \left( \overline{D_1} \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |U_2^n| \overline{D_2}^{-1} \right)_{ijk}^{-1} \delta_y (\overline{D_2} \delta_y d_t C_h^n) \right) \right) \right]_{ijk} \\ & + (\Delta t)^3 \left\{ \left( 1 + \frac{h}{2} |u_1^{n+1}| \overline{D_1}^{-1} \right)_{ijk}^{-1} \delta_x (\overline{D_1} \delta_x (\beta^{-1}(c^{n+1}) \left( 1 + \frac{h}{2} |u_2^{n+1}| \overline{D_2}^{-1} \right)_{ijk}^{-1} \delta_y (\overline{D_2} \delta_y \beta^{-1}(c^{n+1}) \right. \right. \\ & \cdot \left. \left. \left( 1 + \frac{h}{2} |u_3^{n+1}| \overline{D_3}^{-1} \right)_{ijk}^{-1} \delta_z (\overline{D_3} \delta_z d_t c^n) \right) \right) \right) \right\} - \left( 1 + \frac{h}{2} |U_1^n| \overline{D_1}^{-1} \right)_{ijk}^{-1} \delta_x \\ & \cdot \left( \overline{D_1} \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |U_2^n| \overline{D_2}^{-1} \right)_{ijk}^{-1} \delta_y (\overline{D_2} \delta_y \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |U_3^n| \overline{D_3}^{-1} \right)_{ijk}^{-1} \right. \right. \\ & \left. \left. \delta_z (\overline{D_3} \delta_z d_t C_h^n) \right) \right) \right) \right\} + \varepsilon_{1,ijk}^{n+1}, 1 \leq i, j, k \leq N-1, \tag{17a} \end{aligned}$$

$$\xi_{ijk}^{n+1} = 0, X_{ijk} \in \partial\Omega_h, \tag{17b}$$

where  $|\varepsilon_{1,ijk}^{n+1}| \leq M (\Delta t + h^2)$ .

Next, consider the fluid equation. For Equations (11)-(13), dispel  $H_h^{n+1/3}$  and  $H_h^{n+2/3}$ , and we get the following equivalent form:

$$\begin{aligned}
 & S_{s,ijk} \frac{H_{h,ijk}^{n+1} - H_{h,ijk}^n}{\Delta t} - \left\{ \delta_x^-(K_1(C_h^n) \delta_x H_h^{n+1})_{ijk} + \delta_y^-(K_2(C_h^n) \delta_y H_h^{n+1})_{ijk} + \delta_z^-(K_3(C_h^n) \delta_z H_h^{n+1})_{ijk} \right. \\
 & = -\eta \psi_{ijk} \frac{C_{h,ijk}^{n+1} - C_{h,ijk}^n}{\Delta t} + \frac{\rho(C_{h,ijk}^n)}{\rho_0} q_{ijk}^n + \eta \delta_z^-(K_3(C_h^n) C_h^n)_{ijk} \\
 & - (\Delta t)^2 \left\{ \delta_x^-(K_1(C_h^n) \delta_x (S_s^{-1} \delta_y^-(K_2(C_h^n) \delta_y d_t H_h^n)))_{ijk} \right. \\
 & \left. + \delta_x^-(K_1(C_h^n) \delta_x (S_s^{-1} \delta_z^-(K_3(C_h^n) \delta_z d_t H_h^n)))_{ijk} + \delta_y^-(K_2(C_h^n) \delta_y (S_s^{-1} \delta_z^-(K_3(C_h^n) \delta_z d_t H_h^n)))_{ijk} \right\} \\
 & + (\Delta t)^3 \left\{ \delta_x^-(K_1(C_h^n) \delta_x (S_s^{-1} \delta_y^-(K_2(C_h^n) \delta_y (S_s^{-1} \delta_z^-(K_3(C_h^n) \delta_z d_t H_h^n))))_{ijk} \right\}, 1 \leq i, j, k \leq N-1,
 \end{aligned} \tag{18a}$$

$$H_{h,ijk}^{n+1} = h_{ijk}^{n+1}, X_{ijk} \in \partial\Omega_h. \tag{18b}$$

From Equation (1) ( $t = t^{n+1}$ ) and (18) we have the fluid error equations.

$$\begin{aligned}
 & S_{s,ijk} \frac{\pi_{ijk}^{n+1} - \pi_{ijk}^n}{\Delta t} - \left\{ \delta_x^-(K_1(C_h^n) \delta_x \pi^{n+1})_{ijk} + \delta_y^-(K_2(C_h^n) \delta_y \pi^{n+1})_{ijk} + \delta_z^-(K_3(C_h^n) \delta_z \pi^{n+1})_{ijk} \right\} \\
 & = \nabla_h \left( \left[ K(c^{n+1}) - K(C_h^n) \right] \nabla_h H^{n+1} \right)_{ijk} - \eta \psi_{ijk} \frac{\xi_{ijk}^{n+1} - \xi_{ijk}^n}{\Delta t} + \left[ \frac{\rho(c_{ijk}^{n+1})}{\rho_0} q_{ijk}^{n+1} - \frac{\rho(C_{h,ijk}^n)}{\rho_0} q_{ijk}^n \right] \\
 & + \eta \left[ \delta_z^-(K_3(c^{n+1}) c^{n+1})_{ijk} - \delta_z^-(K_3(C_h^n) C_h^n)_{ijk} \right] \\
 & - (\Delta t)^2 \left\{ \left[ \delta_x^-(K_1(c^{n+1}) \delta_x (S_s^{-1} \delta_y^-(K_2(c^{n+1}) \delta_y d_t H^n)))_{ijk} \right. \right. \\
 & \left. - \delta_x^-(K_1(C_h^n) \delta_x (S_s^{-1} \delta_y^-(K_2(C_h^n) \delta_y d_t H^n)))_{ijk} \right] + \left[ \delta_x^-(K_1(c^{n+1}) \delta_x (S_s^{-1} \delta_z^-(K_3(c^{n+1}) \delta_z d_t H^n)))_{ijk} \right. \\
 & \left. - \delta_x^-(K_1(C_h^n) \delta_x (S_s^{-1} \delta_z^-(K_3(C_h^n) \delta_z d_t H^n)))_{ijk} \right] + \left[ \delta_y^-(K_2(c^{n+1}) \delta_y (S_s^{-1} \delta_z^-(K_3(c^{n+1}) \delta_z d_t H^n)))_{ijk} \right. \\
 & \left. - \delta_y^-(K_2(C_h^n) \delta_y (S_s^{-1} \delta_z^-(K_3(C_h^n) \delta_z d_t H^n)))_{ijk} \right] \right\} \\
 & + (\Delta t)^3 \left\{ \delta_x^-(K_1(c^{n+1}) \delta_x (S_s^{-1} \delta_y^-(K_2(c^{n+1}) \delta_y (S_s^{-1} \delta_z^-(K_3(c^{n+1}) \delta_z d_t H^n))))_{ijk} \right. \\
 & \left. - \delta_x^-(K_1(C_h^n) \delta_x (S_s^{-1} \delta_y^-(K_2(C_h^n) \delta_y (S_s^{-1} \delta_z^-(K_3(C_h^n) \delta_z d_t H^n))))_{ijk} \right\} + \varepsilon_{2,ijk}^{n+1},
 \end{aligned} \tag{19a}$$

$1 \leq i, j, k \leq N-1,$

$$\pi_{ijk}^{n+1} = 0, X_{ijk} \in \partial\Omega_h, \tag{19b} \quad \text{where}$$

where  $|\varepsilon_{2,ijk}^{n+1}| \leq M(\Delta t + h^2).$

$$\|\pi^n\|_{1,\infty}^2 = \|\pi^n\|_{0,\infty}^2 + \|\nabla_h \pi^n\|_{0,\infty}^2, \dots$$

We shall introduce the induction hypothesis:

$$\sup_{0 \leq n \leq L} \max \left\{ \|\pi^n\|_{1,\infty}, \|\xi^n\|_{1,\infty} \right\} \rightarrow 0, (h, \Delta t) \rightarrow 0, \tag{20}$$

We consider fluid error Equation (19). Test error Equation (19) against  $\delta_t \pi_{ijk}^{n+1} = \pi_{ijk}^{n+1} - \pi_{ijk}^n$  and summing it up by parts, we have

$$\begin{aligned}
 & \langle S_s d_t \pi^n, d_t \pi^n \rangle \Delta t + \frac{1}{2} \left\{ \left[ \langle K_1(C_h^n) \delta_x \pi^{n+1}, \delta_x \pi^{n+1} \rangle + \langle K_2(C_h^n) \delta_y \pi^{n+1}, \delta_y \pi^{n+1} \rangle \right. \right. \\
 & \left. \left. + \langle K_3(C_h^n) \delta_z \pi^{n+1}, \delta_z \pi^{n+1} \rangle \right] - \left[ \langle K_1(C_h^n) \delta_x \pi^n, \delta_x \pi^n \rangle + \langle K_2(C_h^n) \delta_y \pi^n, \delta_y \pi^n \rangle + \langle K_3(C_h^n) \delta_z \pi^n, \delta_z \pi^n \rangle \right] \right\} \\
 & \leq \left\langle \nabla_h \left( [K(c^{n+1}) - K(C_h^n)] \nabla_h H^{n+1} \right), d_t \pi^n \right\rangle \Delta t - \eta \langle \psi d_t \xi^n, d_t \pi^n \rangle \Delta t \\
 & + \left\langle \frac{\rho(c^{n+1})}{\rho_0} q^{n+1} - \frac{\rho(C_h^n)}{\rho_0} q^n, d_t \pi^n \right\rangle \Delta t \\
 & + \eta \left\langle \delta_z (K_3(c^{n+1})c^{n+1}) - \delta_z (K_3(C_h^n)C_h^n), d_t \pi^n \right\rangle \Delta t \\
 & - (\Delta t)^2 \left\{ \left\langle \delta_x (K_1(c^{n+1})) \delta_x (S_s^{-1} \delta_y (K_2(c^{n+1}) \delta_y d_t H^n)) \right\rangle \right. \\
 & \left. - \delta_x (K_1(C_h^n) \delta_x (S_s^{-1} \delta_y (K_2(C_h^n) \delta_y d_t H^n))) \right\rangle, d_t \pi^n > \Delta t + \dots \} \\
 & + (\Delta t)^3 \left\langle \delta_x (K_1(c^{n+1}) \delta_x (S_s^{-1} \delta_y (K_2(c^{n+1}) \delta_y (S_s^{-1} \delta_z (K_3(c^{n+1}) \delta_z d_t H^n)))) \right\rangle \\
 & \left. - \delta_x (K_1(C_h^n) \delta_x (S_s^{-1} \delta_y (K_2(C_h^n) \delta_y (S_s^{-1} \delta_z (K_3(C_h^n) \delta_z d_t H^n)))) \right\rangle, d_t \pi^n \right\rangle \Delta t + \langle \varepsilon_2^{n+1}, d_t \pi^n \rangle \Delta t. \tag{21}
 \end{aligned}$$

Now we estimate the terms on the right-hand side of (21).

$$\langle \nabla_h \left( [K(c^{n+1}) - K(C_h^n)] \nabla_h H^{n+1} \right), d_t \pi^n \rangle > \Delta t \tag{22a}$$

$$\leq M \left\{ \|\nabla_h \xi^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \pi^n\|^2 \Delta t,$$

$$-\eta \langle \psi d_t \xi^n, d_t \pi^n \rangle \Delta t \tag{22b}$$

$$\leq M \|d_t \xi^n\|^2 \Delta t + \varepsilon \|d_t \pi^n\|^2 \Delta t,$$

$$\left\langle \frac{\rho(c^{n+1})}{\rho_0} q^{n+1} - \frac{\rho(C_h^n)}{\rho_0} q^n, d_t \pi^n \right\rangle > \Delta t \tag{22c}$$

$$\leq M \left\{ \|\xi^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \pi^n\|^2 \Delta t,$$

$$\eta \left\langle \delta_z (K_3(c^{n+1})c^{n+1}) - \delta_z (K_3(C_h^n)C_h^n), d_t \pi^n \right\rangle \Delta t \tag{22d}$$

$$\leq M \left\{ \|\nabla_h \xi^n\|^2 + \|\xi^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \pi^n\|^2 \Delta t,$$

For the fifth term on the right-hand side of (21).

$$\begin{aligned}
 & -(\Delta t)^3 \left\langle \delta_x (K_1(c^{n+1})) \delta_x (S_s^{-1} \delta_y (K_2(c^{n+1}) \delta_y (S_s^{-1} \delta_z (K_3(c^{n+1}) \delta_z d_t H^n)))) \right\rangle \\
 & - \delta_x (K_1(C_h^n) \delta_x (S_s^{-1} \delta_y (K_2(C_h^n) \delta_y (S_s^{-1} \delta_z (K_3(C_h^n) \delta_z d_t H^n)))) \right\rangle, d_t \pi^n > \Delta t \\
 & = -(\Delta t)^3 \left\langle \delta_x (K_1(C_h^n) \delta_x (S_s^{-1} \delta_y (K_2(C_h^n) \delta_y d_t \pi^n))) \right\rangle, d_t \pi^n \tag{23} \\
 & + \left\langle \delta_x (K_1(C_h^n) \delta_x (S_s^{-1} \delta_y ([K_2(c^{n+1}) - K_2(C_h^n)] \delta_y d_t H^n))) \right\rangle, d_t \pi^n \right\rangle \\
 & + \left\langle \delta_x ([K_1(c^{n+1}) - K_1(C_h^n)] \delta_x (S_s^{-1} \delta_y (K_2(c^{n+1}) \delta_y d_t H^n))) \right\rangle, d_t \pi^n \right\rangle.
 \end{aligned}$$

For the first term on the right-hand side of (23), though the operators  $-\delta_x (K \delta_x), -\delta_y (K \delta_y), \dots$  are self-conjugate, positive definite and bounded, space region is cubic. However, their products are generally incommutative.

Noting that

$$\delta_x \delta_y = \delta_y \delta_x, \delta_x \delta_y^- = \delta_y^- \delta_x, \delta_x^- \delta_y = \delta_y \delta_x^-, \delta_x^- \delta_y^- = \delta_y^- \delta_x^-,$$

we have



$$\begin{aligned}
 & -(\Delta t)^3 \left\langle \left\langle \delta_x \left( K_1(C_h^n) \delta_x \left( S_s^{-1} \delta_y \left( K_2(C_h^n) \delta_y d_t \pi^n \right) \right) \right) \right\rangle, d_t \pi^n \right\rangle \\
 & = -(\Delta t)^3 \sum_{i,j,k=1}^N \left\{ K_1(C_h^n)_{i+1/2,jk} K_2(C_h^n)_{i,j+1/2,k} S_{s,ijk}^{-1} \left[ \delta_x \delta_y d_t \pi_{ijk}^n \right]^2 + \left[ K_2(C_h^n)_{i,j+1/2,k} \cdot \delta_y \left( S_{s,ijk}^{-1} K_1(C_h^n)_{i+1/2,jk} \right) \delta_x d_t \pi_{ijk}^n \right. \right. \\
 & + S_{s,ijk}^{-1} K_1(C_h^n)_{i+1/2,jk} \cdot \delta_x K_2(C_h^n)_{i,j+1/2,k} \cdot \delta_y d_t \pi_{ijk}^n + K_2(C_h^n)_{i,j+1/2,k} K_1(C_h^n)_{i+1/2,jk} \cdot \delta_x S_{s,ijk}^{-1} \left. \right] \delta_x \delta_y d_t \pi_{ijk}^n \\
 & + \left[ \delta_x K_2(C_h^n)_{i,j+1/2,k} \cdot \delta_y \left( S_{s,ijk}^{-1} K_1(C_h^n)_{i+1/2,jk} \right) + K_2(C_h^n)_{i,j+1/2,k} \cdot \right. \\
 & \left. \delta_y \left( \delta_x S_{s,ijk}^{-1} \cdot K_1(C_h^n)_{i+1/2,jk} \right) \right] \delta_x d_t \pi_{ijk}^n \cdot \delta_y d_t \pi_{ijk}^n \Big\} h^3. \tag{24}
 \end{aligned}$$

From induction hypothesis (20) we learn that  $K_1(C_h^n), K_2(C_h^n), \delta_x K_1(C_h^n), \delta_y (S_s^{-1} K_1(C_h^n)) \dots$  are bounded. To the first and second terms of expression

(24), the positive definite property of  $K_1, K_2, S_s^{-1}$  should be applied, and high-order difference term  $\delta_x \delta_y d_t \pi_{ijk}^n$  should be separated. By using Cauchy inequality to eliminate the terms concerned, we can get

$$\begin{aligned}
 & -(\Delta t)^3 \sum_{i,j,k=1}^N \left\{ \left[ K_1(C_h^n)_{i+1/2,jk} K_2(C_h^n)_{i,j+1/2,k} S_{s,ijk}^{-1} \left[ \delta_x \delta_y d_t \pi_{ijk}^n \right]^2 + \left[ K_2(C_h^n)_{i,j+1/2,k} \right. \right. \right. \\
 & \cdot \delta_y \left( S_{s,ijk}^{-1} K_1(C_h^n)_{i+1/2,jk} \right) \delta_x d_t \pi_{ijk}^n + S_{s,ijk}^{-1} K_1(C_h^n)_{i+1/2,jk} \cdot \delta_x K_2(C_h^n)_{i,j+1/2,k} \cdot \delta_y d_t \pi_{ijk}^n \\
 & + K_2(C_h^n)_{i,j+1/2,k} K_1(C_h^n)_{i+1/2,jk} \cdot \delta_x S_{s,ijk}^{-1} \left. \right] \delta_x \delta_y d_t \pi_{ijk}^n \Big\} h^3 \leq -\frac{1}{2} K_*^2 (S_s^*)^{-1} (\Delta t)^3 \sum_{i,j,k=1}^N \left[ \delta_x \delta_y d_t \pi_{ijk}^n \right]^2 h^3 \\
 & + M \left\{ \left\| \delta_x d_t \pi^n \right\|^2 + \left\| \delta_y d_t \pi^n \right\|^2 \right\} (\Delta t)^3 \leq -\frac{1}{2} K_*^2 (S_s^*)^{-1} (\Delta t)^3 \sum_{i,j,k=1}^N \left[ \delta_x \delta_y d_t \pi_{ijk}^n \right]^2 h^3 + M \left\{ \left\| \nabla_h \pi^{n+1} \right\|^2 + \left\| \nabla_h \pi^n \right\|^2 \right\} \Delta t. \tag{25a}
 \end{aligned}$$

For the third term of (24), we have

$$\begin{aligned}
 & -(\Delta t)^3 \sum_{i,j,k=1}^N \left\{ \left[ \delta_x K_2(C_h^n)_{i,j+1/2,k} \cdot \delta_y \left( S_{s,ijk}^{-1} K_1(C_h^n)_{i+1/2,jk} \right) + K_2(C_h^n)_{i,j+1/2,k} \right. \right. \\
 & \cdot \delta_y \left( \delta_x S_{s,ijk}^{-1} \cdot K_1(C_h^n)_{i+1/2,jk} \right) \left. \right] \delta_x d_t \pi_{ijk}^n \cdot \delta_y d_t \pi_{ijk}^n \Big\} h^3 \\
 & \leq M \left\{ \left\| \nabla_h \pi^{n+1} \right\|^2 + \left\| \nabla_h \pi^n \right\|^2 \right\} \Delta t. \tag{25b}
 \end{aligned}$$

Similarly, for the other terms, we can obtain

$$\begin{aligned}
 & -(\Delta t)^3 \left\langle \left\langle \delta_x \left( K_1(c^{n+1}) \delta_x \left( S_s^{-1} \delta_y \left( K_2(c^{n+1}) \delta_y d_t H^n \right) \right) \right) - \delta_x \left( K_1(C_h^n) \delta_x \left( S_s^{-1} \delta_y \left( K_2(C_h^n) \delta_y d_t H_h^n \right) \right) \right) \right\rangle, d_t \pi^n \right\rangle + \dots \\
 & + \left\langle \delta_y \left( K_2(c^{n+1}) \delta_y \left( S_s^{-1} \delta_z \left( K_2(c^{n+1}) \delta_z d_t H^n \right) \right) \right), \dots \right\rangle \leq M \left\{ \left\| \nabla_h \pi^{n+1} \right\|^2 + \left\| \nabla_h \pi^n \right\|^2 + \left\| \xi^n \right\|^2 + (\Delta t)^2 \right\} \Delta t. \tag{26}
 \end{aligned}$$

Now, we consider the sixth term of the right-hand side of (21).

$$\begin{aligned}
 & (\Delta t)^4 \left\langle \delta_x \left( K_1(c^{n+1}) \delta_x \left( S_s^{-1} \delta_y \left( K_2(c^{n+1}) \delta_y \left( S_s^{-1} \delta_z \left( K_3(c^{n+1}) \delta_z d_t H^n \right) \right) \right) \right) \right) \right\rangle \\
 & - \delta_x \left( K_1(C_h^n) \delta_x \left( S_s^{-1} \delta_y \left( K_2(C_h^n) \delta_y \left( S_s^{-1} \delta_z \left( K_3(C_h^n) \delta_z d_t H_h^n \right) \right) \right) \right) \right) \Big\rangle, d_t \pi^n \Big\rangle \\
 & \leq -\frac{1}{2} K_*^3 (S_s^*)^{-2} (\Delta t)^4 \sum_{i,j,k=1}^N \left[ \delta_x \delta_y \delta_z d_t \pi_{ijk}^n \right]^2 h^3 + M \left\{ \left\| \nabla_h \pi^{n+1} \right\|^2 + \left\| \nabla_h \pi^n \right\|^2 + \left\| \xi^n \right\|^2 + (\Delta t)^2 \right\} \Delta t. \tag{27}
 \end{aligned}$$

For the last term on the right-hand side of (21).

$$\langle \varepsilon_2^{n+1}, d_t \pi^n \rangle \Delta t \leq M \left\{ \|\nabla_h \pi^{n+1}\|^2 + \|\nabla_h \pi^n\|^2 + \|\xi^n\|^2 + (\Delta t)^2 \right\} \Delta t. \tag{28}$$

From (21)-(28) we can obtain

$$\begin{aligned} & S_s^* \|d_t \pi^n\|^2 \Delta t + \frac{1}{2} \left\{ \langle K(C_h^n) \nabla_h \pi^{n+1}, \nabla_h \pi^{n+1} \rangle - \langle K(C_h^n) \nabla_h \pi^n, \nabla_h \pi^n \rangle \right\} \\ & \leq M \left\{ \|\nabla_h \pi^{n+1}\|^2 + \|\nabla_h \pi^n\|^2 + \|\xi^n\|^2 + \|\nabla_h \xi^n\|^2 + \|d_t \xi^n\|^2 + h^4 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \pi^n\|^2 \Delta t. \end{aligned} \tag{29}$$

Next, consider the concentration error equation. Test error Equation (17) against  $\delta_t \xi^{n+1} = \xi_{ijk}^{n+1} - \xi_{ijk}^n$  and sum-

$$\begin{aligned} & \langle \beta(C_h^n) d_t \xi^n, d_t \xi^n \rangle \Delta t + \left\{ \left\langle \bar{D}_1 \delta_x \xi^{n+1}, \delta_x \left[ \left( 1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1} \right)^{-1} (\xi^{n+1} - \xi^n) \right] \right\rangle \right. \\ & + \left\langle \bar{D}_2 \delta_y \xi^{n+1}, \delta_y \left[ \left( 1 + \frac{h}{2} |u_2^{n+1}| \bar{D}_2^{-1} \right)^{-1} (\xi^{n+1} - \xi^n) \right] \right\rangle + \left\langle \bar{D}_3 \delta_z \xi^{n+1}, \delta_z \left[ \left( 1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1} \right)^{-1} (\xi^{n+1} - \xi^n) \right] \right\rangle \left. \right\} \\ & = \left\langle \delta_{U_{1,x}^n} C_h^n - \delta_{U_{1,x}^n} c^{n+1}, d_t \xi^n \right\rangle + \left\langle \delta_{U_{2,y}^n} C_h^n - \delta_{U_{2,y}^n} c^{n+1}, d_t \xi^n \right\rangle + \left\langle \delta_{U_{3,z}^n} C_h^n - \delta_{U_{3,z}^n} c^{n+1}, d_t \xi^n \right\rangle \left. \right\} \Delta t \\ & + \left\{ \left\langle \left[ \left( 1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1} \right)^{-1} - \left( 1 + \frac{h}{2} |u_1^n| \bar{D}_1^{-1} \right)^{-1} \right] \delta_x (\bar{D}_1 \delta_x C_h^{n+1}), d_t \xi^n \right\rangle \right. \\ & \left\langle \left[ \left( 1 + \frac{h}{2} |u_2^{n+1}| \bar{D}_2^{-1} \right)^{-1} - \left( 1 + \frac{h}{2} |u_2^n| \bar{D}_2^{-1} \right)^{-1} \right] \delta_y (\bar{D}_2 \delta_y C_h^{n+1}), d_t \xi^n \right\rangle \\ & \left. \left\langle \left[ \left( 1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1} \right)^{-1} - \left( 1 + \frac{h}{2} |u_3^n| \bar{D}_3^{-1} \right)^{-1} \right] \delta_z (\bar{D}_3 \delta_z C_h^{n+1}), d_t \xi^n \right\rangle \right\} \Delta t \\ & + \left\langle q^{n+1} (C^{*,n+1} - C^{n+1}) - q^n (C^{*,n} - C^n), d_t \xi^n \right\rangle \Delta t \\ & - (\Delta t)^3 \left\{ \left\langle \left( 1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1} \right)^{-1} \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |u_3^n| \bar{D}_3^{-1} \right)^{-1} \delta_z (\bar{D}_3 \delta_z d_t \xi^n) \right) \right), d_t \xi^n \right\rangle + \dots \right\} \\ & + (\Delta t)^4 \left( 1 + \frac{h}{2} |u_1^n| \bar{D}_1^{-1} \right)^{-1} \\ & \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1} \right)^{-1} \delta_y \left( \bar{D}_2 \delta_y \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2} |u_3^n| \bar{D}_3^{-1} \right)^{-1} \delta_z (\bar{D}_3 \delta_z d_t \xi^n) \right) \right) \right) \right) \right) \left. \right\} + \dots \left. \right\} \\ & + \langle \varepsilon_1^{n+1}, d_t \xi^n \rangle \Delta t \end{aligned} \tag{30}$$

First, we estimate the second term on the left-hand side of (30).

$$\begin{aligned} & \left\langle \bar{D}_1 \delta_x \xi^{n+1}, \delta_x \left[ \left( 1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1} \right)^{-1} (\xi^{n+1} - \xi^n) \right] \right\rangle \geq \frac{1}{2} \left\{ \left\langle \bar{D}_1 \delta_x \xi^{n+1}, \left( 1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1} \right)^{-1} \delta_x \xi^{n+1} \right\rangle \right. \\ & \left. - \left\langle \bar{D}_1 \delta_x \xi^n, \left( 1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1} \right)^{-1} \delta_x \xi^n \right\rangle \right\} - M \|\nabla_h \xi^{n+1}\|^2 \Delta t - \varepsilon \|d_t \xi^n\|^2 \Delta t. \end{aligned} \tag{31a}$$

Similarly,

$$\begin{aligned} & \left\langle \bar{D}_2 \delta_y \xi^{n+1}, \delta_y \left[ \left( 1 + \frac{h}{2} |u_2^{n+1}| \bar{D}_2^{-1} \right)^{-1} (\xi^{n+1} - \xi^n) \right] \right\rangle \\ & \geq \frac{1}{2} \left\{ \left\langle \bar{D}_2 \delta_y \xi^{n+1}, \left( 1 + \frac{h}{2} |u_2^{n+1}| \bar{D}_2^{-1} \right)^{-1} \delta_y \xi^{n+1} \right\rangle - \left\langle \bar{D}_2 \delta_y \xi^n, \left( 1 + \frac{h}{2} |u_2^{n+1}| \bar{D}_2^{-1} \right)^{-1} \delta_y \xi^n \right\rangle \right\} - M \|\nabla_h \xi^{n+1}\|^2 \Delta t - \varepsilon \|d_t \xi^n\|^2 \Delta t. \end{aligned} \tag{31b}$$

$$\begin{aligned} & \left\langle \bar{D}_3 \delta_z \xi^{n+1}, \delta_z \left[ \left( 1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1} \right)^{-1} (\xi^{n+1} - \xi^n) \right] \right\rangle \\ & \geq \frac{1}{2} \left\{ \left\langle \bar{D}_3 \delta_z \xi^{n+1}, \left( 1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1} \right)^{-1} \delta_z \xi^{n+1} \right\rangle - \left\langle \bar{D}_3 \delta_z \xi^n, \left( 1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1} \right)^{-1} \delta_z \xi^n \right\rangle \right\} - M \|\nabla_h \xi^{n+1}\|^2 \Delta t - \varepsilon \|d_t \xi^n\|^2 \Delta t. \end{aligned} \tag{31c}$$

Now, we estimate the terms on the right-hand side of (30). In induction hypothesis (20)  $U^n$  is bounded, so we have

$$\left\langle \delta_{U_1^n, x} C_h^n - \delta_{u_1^{n+1}, x} c^{n+1}, d_t \xi^n \right\rangle \Delta t \leq M \left\{ \|U_1^n - u_1^n\|^2 + \|\nabla_h \xi^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \xi^n\|^2 \Delta t. \tag{32a}$$

Similarly,

$$\begin{aligned} & \left\{ \left\langle \delta_{U_2^n, y} C_h^n - \delta_{u_2^{n+1}, y} c^{n+1}, d_t \xi^n \right\rangle + \left\langle \delta_{U_3^n, z} C_h^n - \delta_{u_3^{n+1}, z} c^{n+1}, d_t \xi^n \right\rangle \right\} \Delta t \\ & \leq M \left\{ \|U_2^n - u_2^n\|^2 + \|U_3^n - u_3^n\|^2 + \|\nabla_h \xi^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \xi^n\|^2 \Delta t. \end{aligned} \tag{32b}$$

For the second term on the right-hand side of (30), we have

$$\begin{aligned} & \left\{ \left\langle \left[ \left( 1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1} \right)^{-1} - \left( 1 + \frac{h}{2} |U_1^n| \bar{D}_1^{-1} \right)^{-1} \right] \delta_x (\bar{D}_1 \delta_x C_h^{n+1}), d_t \xi^n \right\rangle + \dots \right. \\ & \left. \left\langle \left[ \left( 1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1} \right)^{-1} - \left( 1 + \frac{h}{2} |U_3^n| \bar{D}_3^{-1} \right)^{-1} \right] \delta_z (\bar{D}_3 \delta_z C_h^{n+1}), d_t \xi^n \right\rangle \right\} \Delta t \leq M \left\{ \|u^n - U^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \xi^n\|^2 \Delta t. \end{aligned} \tag{33}$$

For the third term, we have

$$\left\langle q^{n+1} (C^{*,n+1} - c^{n+1}) - q^n (C^{*,n} - C^n), d_t \xi^n \right\rangle \Delta t \leq M \left\{ \|\xi^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \xi^n\|^2 \Delta t. \tag{34}$$

We consider the fourth term, and we have

$$\begin{aligned} & -(\Delta t)^3 \left\{ \left\langle \left( 1 + \frac{h}{2} |U_1^n| \bar{D}_1^{-1} \right)^{-1} \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1} (C_h^n) \left( 1 + \frac{h}{2} |U_2^n| \bar{D}_2^{-1} \right)^{-1} \delta_y (\bar{D}_2 \delta_y d_t \xi^n) \right) \right), d_t \xi^n \right\rangle \right. \\ & = -(\Delta t)^3 \sum_{i,j,k=1}^N \left\{ \bar{D}_{1,i+1/2,jk} \bar{D}_{2,i,j+1/2,k} \beta^{-1} (C_{h,ijk}^n) \left( 1 + \frac{h}{2} |U_{1,ijk}^n| \bar{D}_{1,ijk}^{-1} \right)^{-1} \left( 1 + \frac{h}{2} |U_{2,ijk}^n| \bar{D}_{2,ijk}^{-1} \right)^{-1} (\delta_x \delta_y d_t \xi_{ijk}^n)^2 \right. \\ & + \left[ \bar{D}_{2,i,j+1/2,k} \delta_x \bar{D}_{2,i,j+1/2,k} \beta^{-1} (C_{h,ijk}^n) \left( 1 + \frac{h}{2} |U_{2,ijk}^n| \bar{D}_{2,ijk}^{-1} \right)^{-1} \left( 1 + \frac{h}{2} |U_{1,ijk}^n| \bar{D}_{1,ijk}^{-1} \right)^{-1} \delta_y d_t \xi_{ijk}^n + \bar{D}_{2,i,j+1/2,k} \right. \\ & \left. \left. \delta_y \left[ \bar{D}_{1,i+1/2,jk} \beta^{-1} (C_{h,ijk}^n) \left( 1 + \frac{h}{2} |U_{2,ijk}^n| \bar{D}_{2,ijk}^{-1} \right)^{-1} \left( 1 + \frac{h}{2} |U_{1,ijk}^n| \bar{D}_{1,ijk}^{-1} \right)^{-1} \right] \delta_x d_t \xi_{ijk}^n + \dots \right] \delta_x \delta_y d_t \xi_{ijk}^n + \dots \right\} h^3. \end{aligned}$$

On positive definite condition:

$$\psi_* D_* \leq \bar{D}_i \leq \psi^* D^*, 0 < \beta_* \leq \beta(C) \leq \beta^*, 0 < (\beta^*)^{-1} \leq \beta^{-1}(C) \leq (\beta_*)^{-1}.$$

In induction hypothesis (20)  $U^n$  is bounded, so we have  $(1 + h/2|U_\alpha^n|\bar{D}_\alpha^{-1})^{-1} \geq b_0 > 0, \alpha = 1, 2, 3,$

$$\begin{aligned} & -(\Delta t)^3 \left\langle \left( \left( 1 + \frac{h}{2}|U_1^n|\bar{D}_1^{-1} \right)^{-1} \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2}|U_2^n|\bar{D}_2^{-1} \right)^{-1} \delta_y (\bar{D}_2 \delta_y d_t \xi^n) \right) \right) \right), d_t \xi^n \right\rangle \\ & \leq -\frac{(\Delta t)^3}{2} (\psi_* D_*)^2 (\beta^*)^{-1} b_0^2 \|\delta_x \delta_y d_t \xi^n\|^2 + M (\Delta t)^3 \left\{ \|\nabla_h d_t \xi^n\|^2 + \|d_t \xi^n\|^2 \right\}. \end{aligned}$$

Thus, for the fourth term we can obtain

$$\begin{aligned} & -(\Delta t)^3 \left\langle \left( \left( 1 + \frac{h}{2}|U_1^n|\bar{D}_1^{-1} \right)^{-1} \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2}|U_2^n|\bar{D}_2^{-1} \right)^{-1} \delta_y (\bar{D}_2 \delta_y d_t \xi^n) \right) \right) \right), d_t \xi^n \right\rangle + \dots \\ & + \left\langle \left( \left( 1 + \frac{h}{2}|u_1^{n+1}|\bar{D}_1^{-1} \right)^{-1} - \left( 1 + \frac{h}{2}|U_1^n|\bar{D}_1^{-1} \right)^{-1} \right) \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1}(c^{n+1}) \left( 1 + \frac{h}{2}|u_2^{n+1}|\bar{D}_2^{-1} \right)^{-1} \delta_y (\bar{D}_2 \delta_y d_t c^n) \right) \right) \right), d_t \xi^n \right\rangle \quad (35a) \\ & \leq -\frac{(\Delta t)^3}{2} (\psi_* D_*)^2 (\beta^*)^{-1} b_0^2 \|\delta_x \delta_y d_t \xi^n\|^2 + M \left\{ \|\nabla_h \xi^{n+1}\|^2 + \|\nabla_h \xi^n\|^2 + \|\xi^{n+1}\|^2 + \|\xi^n\|^2 \right\} \Delta t. \end{aligned}$$

Similarly, for the fifth and sixth terms we have

$$\begin{aligned} & -(\Delta t)^3 \left\langle \left( \left( 1 + \frac{h}{2}|U_1^n|\bar{D}_1^{-1} \right)^{-1} \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2}|U_3^n|\bar{D}_3^{-1} \right)^{-1} \delta_z (\bar{D}_3 \delta_z d_t \xi^n) \right) \right) \right), d_t \xi^n \right\rangle + \dots \quad (35b) \\ & \leq -\frac{(\Delta t)^3}{2} (\psi_* D_*)^2 (\beta^*)^{-1} b_0^2 \left\{ \|\delta_x \delta_y d_t \xi^n\|^2 + \|\delta_x \delta_z d_t \xi^n\|^2 + \|\delta_y \delta_z d_t \xi^n\|^2 \right\} \\ & + M \left\{ \|\nabla_h \xi^{n+1}\|^2 + \|\nabla_h \xi^n\|^2 + \|\xi^{n+1}\|^2 + \|\xi^n\|^2 \right\} \Delta t. \end{aligned}$$

For the seventh term we have

$$\begin{aligned} & (\Delta t)^4 \left\langle \left( \left( 1 + \frac{h}{2}|U_1^n|\bar{D}_1^{-1} \right)^{-1} \delta_x \left( \bar{D}_1 \delta_x \left( \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2}|U_2^n|\bar{D}_2^{-1} \right)^{-1} \delta_y \left( \bar{D}_2 \delta_y \beta^{-1}(C_h^n) \left( 1 + \frac{h}{2}|U_3^n|\bar{D}_3^{-1} \right)^{-1} \delta_z (\bar{D}_3 \delta_z d_t \xi^n) \right) \right) \right) \right)_{ijk} \right), d_t \xi^n \right\rangle + \dots \quad (36) \\ & \leq -\frac{(\Delta t)^4}{2} (\psi_* D_*)^3 (\beta^*)^{-2} b_0^2 \|\delta_x \delta_y \delta_z d_t \xi^n\|^2 + M \left\{ \|\nabla_h \xi^{n+1}\|^2 + \|\nabla_h \xi^n\|^2 + \|\xi^{n+1}\|^2 + \|\xi^n\|^2 \right\} \Delta t. \end{aligned}$$

For the last term

$$\langle \varepsilon_1^{n+1}, d_t \xi^n \rangle \Delta t \leq \varepsilon \|d_t \xi^n\|^2 \Delta t + M \left\{ (\Delta t)^2 + h^4 \right\}. \quad (37)$$

For error Equation (30), from (31)-(37) we can obtain

$$\begin{aligned}
 & \|d_t \xi^n\|^2 \Delta t + \frac{1}{2} \left\{ \left[ \left\langle \bar{D}_1 \delta_x \xi^{n+1}, \left(1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1}\right)^{-1} \delta_x \xi^{n+1} \right\rangle + \left\langle \bar{D}_2 \delta_y \xi^{n+1}, \left(1 + \frac{h}{2} |u_2^{n+1}| \bar{D}_2^{-1}\right)^{-1} \delta_y \xi^{n+1} \right\rangle \right. \right. \\
 & + \left. \left\langle \bar{D}_3 \delta_z \xi^{n+1}, \left(1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1}\right)^{-1} \delta_z \xi^{n+1} \right\rangle \right] - \left[ \left\langle \bar{D}_1 \delta_x \xi^n, \left(1 + \frac{h}{2} |u_1^{n+1}| \bar{D}_1^{-1}\right)^{-1} \delta_x \xi^n \right\rangle \right. \\
 & + \left. \left. \left\langle \bar{D}_2 \delta_y \xi^n, \left(1 + \frac{h}{2} |u_2^{n+1}| \bar{D}_2^{-1}\right)^{-1} \delta_y \xi^n \right\rangle + \left\langle \bar{D}_3 \delta_z \xi^n, \left(1 + \frac{h}{2} |u_3^{n+1}| \bar{D}_3^{-1}\right)^{-1} \delta_z \xi^n \right\rangle \right] \right\} \\
 & \leq M \left\{ \|u^n - U^n\|^2 + \|\nabla_h \xi^{n+1}\|^2 + \|\nabla_h \xi^n\|^2 + \|\xi^{n+1}\|^2 + \|\xi^n\|^2 + (\Delta t)^2 \right\} \Delta t + \varepsilon \|d_t \xi^n\|^2 \Delta t.
 \end{aligned} \tag{38}$$

For fluid error Equation (29), summing over  $0 \leq n \leq L$  and noting that  $\pi^0 = 0$ , we have

$$\begin{aligned}
 & \sum_{n=0}^L \|d_t \pi^n\|^2 \Delta t + \langle K(C_h^L) \nabla_h \pi^{L+1}, \nabla_h \pi^{L+1} \rangle - \langle K(C_h^0) \nabla_h \pi^0, \nabla_h \pi^0 \rangle \\
 & \leq \sum_{n=1}^L \langle [K(C_h^n) - K(C_h^{n-1})] \nabla_h \pi^n, \nabla_h \pi^n \rangle + \sum_{n=0}^L \left\{ \|u^n - U^n\|^2 + \|\nabla_h \xi^{n+1}\|^2 + \|\nabla_h \xi^n\|^2 + \|\xi^{n+1}\|^2 + \|\xi^n\|^2 + (\Delta t)^2 \right\} \Delta t
 \end{aligned} \tag{39}$$

For the first term on the right-hand side of (39) we have

$$\sum_{n=1}^L \langle [K(C_h^n) - K(C_h^{n-1})] \nabla_h E^n, \nabla_h \pi^n \rangle \leq \varepsilon \sum_{n=1}^L \|d_t \xi^{n-1}\|^2 \Delta t + M \sum_{n=1}^L \|\nabla_h \pi^n\|^2 \Delta t. \tag{40}$$

By

$$\|u^n - U^n\|^2 \leq M \left\{ \|\xi^n\|^2 + \|\nabla_h \pi^n\|^2 + h^4 \right\}, \tag{41}$$

we have

$$\sum_{n=0}^L \|d_t \pi^n\|^2 \Delta t + \|\pi^{L+1}\|_1^2 \leq \varepsilon \sum_{n=0}^{L-1} \|d_t \xi^n\|^2 \Delta t + M \left\{ \sum_{n=1}^L [\|\nabla_h \pi^n\|^2 + \|\xi^{n+1}\|_1^2] \Delta t + (\Delta t)^2 + h^4 \right\}. \tag{42}$$

For concentration error Equation (38), summing over  $0 \leq n \leq L$  and noting that  $\xi^0 = 0$ , we can obtain

$$\begin{aligned}
 & \sum_{n=0}^L \|d_t \xi^n\|^2 \Delta t + \frac{1}{2} \left\{ \left[ \left\langle \bar{D}_1 \delta_x \xi^{L+1}, \left(1 + \frac{h}{2} |u_1^{L+1}| \bar{D}_1^{-1}\right)^{-1} \delta_x \xi^{L+1} \right\rangle \right. \right. \\
 & + \left. \left\langle \bar{D}_2 \delta_y \xi^{L+1}, \left(1 + \frac{h}{2} |u_2^{L+1}| \bar{D}_2^{-1}\right)^{-1} \delta_y \xi^{L+1} \right\rangle + \left\langle \bar{D}_3 \delta_z \xi^{L+1}, \left(1 + \frac{h}{2} |u_3^{L+1}| \bar{D}_3^{-1}\right)^{-1} \delta_z \xi^{L+1} \right\rangle \right] \\
 & - \left[ \left\langle \bar{D}_1 \delta_x \xi^0, \left(1 + \frac{h}{2} |u_1^0| \bar{D}_1^{-1}\right)^{-1} \delta_x \xi^0 \right\rangle + \left\langle \bar{D}_2 \delta_y \xi^0, \left(1 + \frac{h}{2} |u_2^0| \bar{D}_2^{-1}\right)^{-1} \delta_y \xi^0 \right\rangle + \left\langle \bar{D}_3 \delta_z \xi^0, \left(1 + \frac{h}{2} |u_3^0| \bar{D}_3^{-1}\right)^{-1} \delta_z \xi^0 \right\rangle \right] \right\} \\
 & \leq \frac{1}{2} \sum_{n=1}^L \left\{ \left\langle \bar{D}_1 \delta_x \xi^n, \left[ \left(1 + \frac{h}{2} |u_1^n| \bar{D}_1^{-1}\right)^{-1} - \left(1 + \frac{h}{2} |u_1^{n-1}| \bar{D}_1^{-1}\right)^{-1} \right] \delta_x \xi^n \right\rangle \right. \\
 & + \left. \left\langle \bar{D}_2 \delta_y \xi^n, \left[ \left(1 + \frac{h}{2} |u_2^n| \bar{D}_2^{-1}\right)^{-1} - \left(1 + \frac{h}{2} |u_2^{n-1}| \bar{D}_2^{-1}\right)^{-1} \right] \delta_y \xi^n \right\rangle \right. \\
 & \left. + \left\langle \bar{D}_3 \delta_z \xi^n, \left[ \left(1 + \frac{h}{2} |u_3^n| \bar{D}_3^{-1}\right)^{-1} - \left(1 + \frac{h}{2} |u_3^{n-1}| \bar{D}_3^{-1}\right)^{-1} \right] \delta_z \xi^n \right\rangle \right\} + M \left\{ \sum_{n=0}^L [\|\nabla_h \pi^n\|^2 + \|\xi^{n+1}\|_1^2] \Delta t + (\Delta t)^2 + h^4 \right\} \Delta t.
 \end{aligned}$$

Then,

$$\begin{aligned} & \sum_{n=0}^L \|d_t \xi^n\|^2 \Delta t + \frac{1}{2} \left\langle \left\langle \bar{D}_1 \delta_x \xi^{L+1}, \left(1 + \frac{h}{2} |u_1^{L+1}| \bar{D}_1^{-1}\right)^{-1} \delta_x \xi^{L+1} \right\rangle \right. \\ & \left. + \left\langle \bar{D}_2 \delta_y \xi^{L+1}, \left(1 + \frac{h}{2} |u_2^{L+1}| \bar{D}_2^{-1}\right)^{-1} \delta_y \xi^{L+1} \right\rangle + \left\langle \bar{D}_3 \delta_z \xi^{L+1}, \left(1 + \frac{h}{2} |u_3^{L+1}| \bar{D}_3^{-1}\right)^{-1} \delta_z \xi^{L+1} \right\rangle \right\} \\ & \leq M \left\{ \sum_{n=0}^L \left[ \|\nabla_h \pi^n\|^2 + \|\xi^{n+1}\|_1^2 \right] \Delta t + (\Delta t)^2 + h^4 \right\} \Delta t. \end{aligned} \tag{43}$$

Combining (42) with (43) it yields

$$\sum_{n=0}^L \left[ \|d_t \xi^n\|^2 + \|d_t \pi^n\|^2 \right] \Delta t + \|\xi^{L+1}\|_1^2 + \|\pi^{L+1}\|_1^2 \leq M \left\{ \sum_{n=0}^L \left[ \|\pi^n\|_1^2 + \|\xi^{n+1}\|_1^2 \right] \Delta t + (\Delta t)^2 + h^4 \right\} \Delta t. \tag{44}$$

Applying discrete Gronwall inequality, we have

$$\sum_{n=0}^L \left[ \|d_t \xi^n\|^2 + \|d_t \pi^n\|^2 \right] \Delta t + \|\xi^{L+1}\|_1^2 + \|\pi^{L+1}\|_1^2 \leq M \left\{ (\Delta t)^2 + h^4 \right\}. \tag{45}$$

It remains to check induction hypothesis (20). First, for  $n = 0$ , since  $\pi^0 = \xi^0 = 0$ , (20) is correct. If  $1 \leq n \leq L$ , (20) holds. From (45) we have  $\|\pi^{L+1}\|_{1,\infty} + \|\xi^{L+1}\|_{1,\infty} \leq Mh^{1/2}$ , then induction hypothesis holds for  $n = L+1$ .

For the first order weighted upwind finite difference fractional steps scheme, we have the following theorem.

Theorem II. Suppose that exact solutions of problem (1)-(5) satisfy condition:

$$H, c \in W^{1,\infty}(W^{1,\infty}) \cap L^\infty(W^{4,\infty}),$$

$$\partial H / \partial t, \partial c / \partial t \in L^\infty(W^{4,\infty}), \partial^2 H / \partial t^2, \partial^2 c / \partial t^2 \in L^\infty(L^\infty).$$

Adopt the first order weighted upwind procedures (8)'-(10)', (11)-(13). Then the following error estimates hold:

$$\begin{aligned} & \|H - H_h\|_{L^\infty(J;h^1)} + \|c - C_h\|_{L^\infty(J;h^1)} + \|d_t(H - H_h)\|_{L^2(J;h^2)} \\ & + \|d_t(c - C_h)\|_{L^2(J;h^2)} \leq M^{**} (\Delta t + h). \end{aligned} \tag{46}$$

### 4. Numerical Simulation Results and Analysis

Considering the complexity of problem, we select Huang-

heyong area of Longkou city as the model area which has 3-dimensional observation grid. This area is on the left bank of Huangshui River neighboring with Bohai in the north and Huangshui River in the east. Its length is 3000 meters and the width is 700 meters. Its average thickness is about 17 or 18 meters. In the upper part of the water-containing layer there is relatively fine sand, and in the lower part—coarse sand with gravel which contains one, two or three layers of mild clay and sludge of different thickness. We decompose this area into three parts according to the permeability. The section graph and plane graph are listed in **Figures 1** and **2**, respectively. The geological parameters are listed in **Table 1**, where No., CP, RWS, SY, DD and ICP denote zone number, coefficients of permeability, rate of water, specific yield, dispersion degree and infiltration coefficient of precipitation.

Let  $h_x = 20$  m,  $h_y = 30$  m,  $h_z = 1$  m. We compare our results, real values and the results of others. A represents the results of Nanjing University [30], and B represents our results. The comparison of graphs of water head and concentration are listed in **Figures 3** and **4**, respectively. The section graphs for water and concentration are listed in **Figures 5** and **6**.

**Table 1. The geological parameters.**

No.	CP (m/d)		RWS (m <sup>-1</sup> )	SY	DD (m)		ICP
	$K_{xx} = K_{yy}$	$K_{zz}$	$S_y$	$S_y$	$\alpha_L$	$\alpha_r$	
A	17	15	$8.0 \times 10^{-5}$	0.075	8.3	0.001	0.3
B	103	22	$1.2 \times 10^{-4}$	0.13	8.3	0.001	0.3
C	7	7	$5.0 \times 10^{-5}$	0.04	0.08	0.0004	0.3
D	63	17	$1.0 \times 10^{-4}$	0.11	0.08	0.0004	0.3

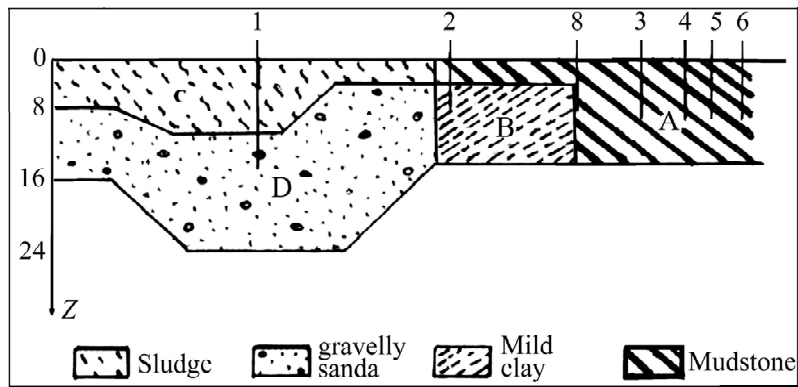


Figure 1. The section graph.

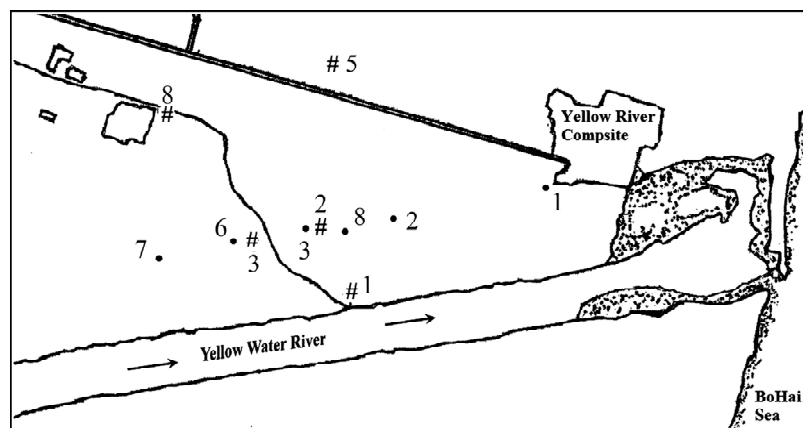


Figure 2. The plane graph.

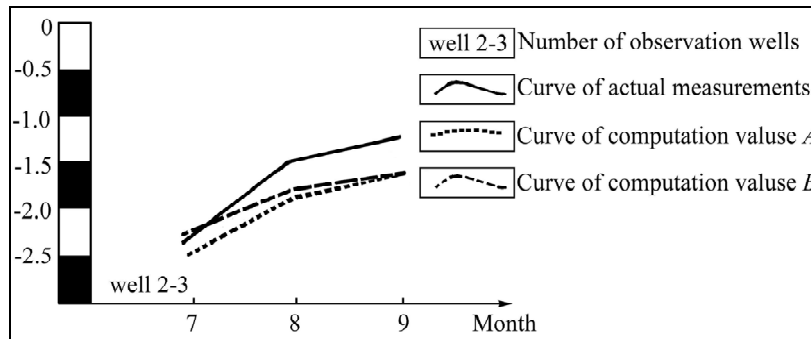


Figure 3. Curves of water level comparison.

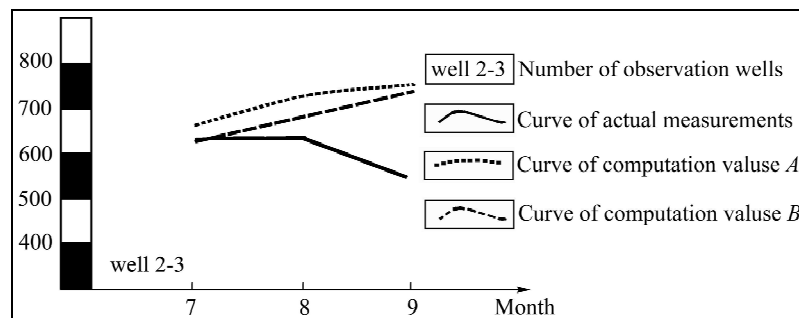


Figure 4. Curves of concentration comparison.

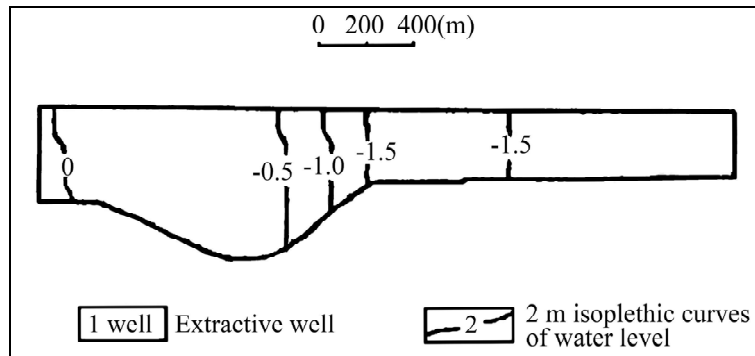


Figure 5. Section graph of water level computation in September.

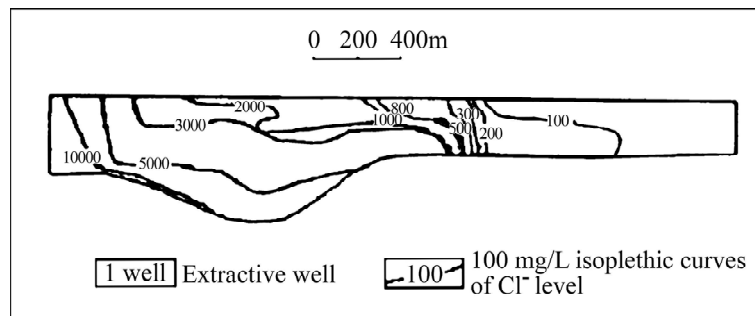


Figure 6. Section graph of Cl<sup>-</sup> concentration in September.

From the above we can see that the computation results are exact, and the algorithm given in this paper is stable and can be used as the algorithm for the simulation of large-scaled problems.

### 5. Consequences of Protection Projects and Applied Modular Form of Project Adjustment

#### 5.1. Consequences of Projection Projects

The main water conservancy works against seawater intrusion include projects for water saving, Yellow River regulation, water retaining and artificial precipitation. Their ultimate goals are to increase water supplies and to decrease the extraction of underground water the production of human and animal needed, so that the descent of underground water level will be slowed down and even underground water be increased. All this is very effective. Up to now, the protection project results are mainly empirical and qualitative. We have not seen publications both in China and abroad about the real salt water and fresh water movement changes after the projects are simulated with computers. There are no publications on the quantitative and comprehensive predictions of various projects. Now we take watersaving project as an example to discuss the predictive result of the projects.

Scheme: Keep the present precipitation level. Take into consideration the effects of water-saving project on seawater intrusion. Take the average precipitation amount

in many years (Refer to “Comprehensive Control Plan Against Seawater Intrusion in Laizhou Bay Area of Shandong Province”). Simulate water levels and changes of salt concentration two months after the peak period (July-August) in the following four conditions: the present pumping out, saving water 10%, saving water 20% and saving water 30%. Water heads and concentrations of some wells at initial time are listed in **Table 2**. The calculation and comparison results are listed in **Tables 3** and **4**. The predictive sections at water saving 20% are listed in **Figures 7** and **8**.

From the above we can see the consequences of water saving projects are remarkable. During raining seasons the underground water level rises again quickly. In dry seasons, its descent is slowed down. So the projects slow down the migration of salt concentration to fresh water

Table 2. The initial values of water head and concentration.

Well No.	Water head (m)	Salt concentration (mg/L)
1-2	-1.01	3667
2-2	-2.20	3000
3-2	-2.77	377
4-2	-3.10	400
5-2	-3.13	98
6-2	-2.87	100

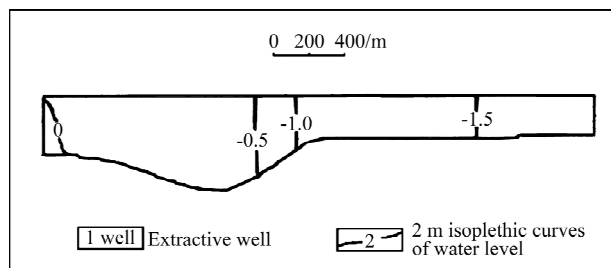


**Table 3. The effects of water saving projects on water head.**

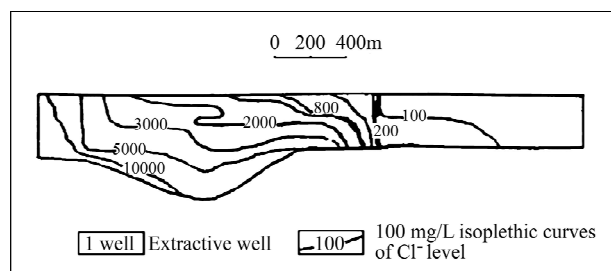
Saving water	Well number, Water head					
	1-2	2-2	3-2	4-2	5-2	6-2
0	-0.45	-1.75	-2.04	-2.42	-2.32	-2.16
10%	-0.34	-1.52	-1.80	-2.14	-2.07	-1.93
20%	-0.23	-1.31	-1.56	-1.87	-1.81	-1.71
30%	-0.12	-1.10	-1.33	-1.60	-1.55	-1.48

**Table 4. The effects of water saving projects on salt concentration.**

Saving water	Well number, Water head					
	1-2	2-2	3-2	4-2	5-2	6-2
0	3871	3044	1521	101	98	99
10%	3753	3088	1507	101	98	99
20%	3725	3032	1493	101	98	99
30%	3696	3027	1479	100	98	100



**Figure 7. The water head prediction at 20% water saving in July-August.**



**Figure 8. The salt concentration prediction at 20% water saving in July-August.**

areas.

### 5.2. Predicting the Consequences of Underground Dam and Tidal Barrage Projects

Underground dams and reservoirs are built with the aim to regulation underground water and prevent seawater intrusion. Underground cut-off walls are built to stop

undercurrent and seawater, since water head is low and the dams are located under the ground, so the stability and safety are high. We can say that the seepage control ability of dams is the key point. Our practice indicates the following four effects. Firstly, underground dams stop undercurrent and increase water supply, playing the role of saving and regulating water. Secondly, they raise underground water level and increase artificial precipitation supply coefficient, playing the role of retaining and supplying water. Thirdly, the upper reaches dams in seawater invaded regions retain and regulate underground water, increase the height of the fresh water heads in upper reaches, relieving the present seawater intrusion and thus playing an important role for seawater invaded regions in lower reaches. Finally, the dams in lower reaches (near the coast) prevent seawater intrusion. Tidal barrages are usually composed of two parts: the part on the ground and the underground base. Our analysis indicates that both parts are very useful. The on-the-ground part prevents seawater coming in with windstorms, while the underground part prevents seawater intrusion in common situations because of its small permeability. The advantages of tidal barrages especially obvious in of windy period.

There usually are two kinds of anti-percolator, namely: lower reaches dam in seawater invaded region, and upper reaches dam in seawater invaded region.

Lower reaches dams should be built on rivers which empty into the sea, or in other places where both salt and fresh water move freely. If a large amount of underground water is pumped out in coastal areas, water level goes down rapidly. When underground water level is lower than the average tidal level, seawater intrusion happens. This is because of the continuity between inland fresh water and seawater. Underground dams reduce greatly or completely stops the permeability of autochthonous layer. Therefore, cut-off walls can reduce the possibility of the seawater in lower reaches intruding inland. Moreover, they can retain and regulate the drainage of underground water. They stop seawater intrusion thanks to the combined actions of their own and fresh water curtain. Underground dams should be located far from the upstream of tides with the consideration of tide actions. Otherwise, tidal barrages should be built whose upper part is barrage and the lower part is underground dam.

As for the upper reaches dams in seawater intruded areas, since the intrusion has occurred, the underground walls must be built at the head of these areas with the aim to retain underground water and increase the fresh water head from upper reaches and to make seawater intrusion stable. This is also useful for inland fresh water areas far from the coast because these dams prevent the decrease of fresh water amount going into the sea, and

thus prevent the descent of underground water level in the upper area of intruded areas. The descent of underground water level accelerates seawater going into the inner part of fresh water areas.

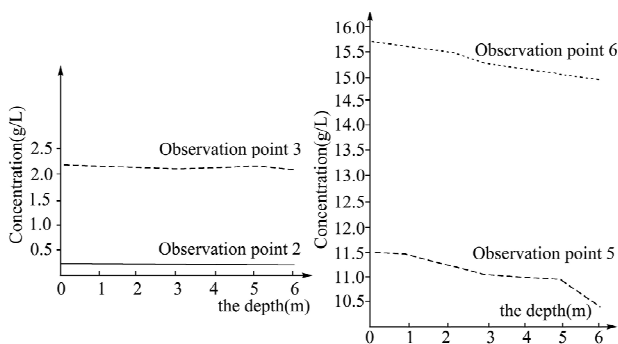
We predicted the effects of the dams on both upper and lower reaches on seawater intrusion. We chose the above-mentioned calculation regions. The results are shown in **Table 5**. **Figure 9** shows the calculated concentration comparison curve. Where A is the depth of the lower reaches dam 0 m. water level of the upper reaches is -1.5 m. B is the depth of lower reaches dam 2m. Water level of the upper reaches is -1 m. C is the depth of lower reaches dam 4 m. Water level of upper reaches is -0.5 m. D is the depth of the lower reaches dam 6 m. Water level of upper reaches is 0 m.

### 5.3. Applied Modular Form of Project Adjustment

We should also apply numerical simulation to make underground water mechanics serve our goal. As for water supply, we should study how to make the limited underground water resources exert the most social and economic benefits, how to limits underground water level descent within our control and how make water supply reach the utmost. As for the protection of natural resources, we should study how to control pollutant discharge and prevent underground water being polluted, and how to keep water quality within the permission of hygienic standards. Here we propose the optimal

**Table 5. Cl<sup>-</sup> concentration computation with the effect of upper reaches and lower reaches dams (after two months).**

Computation condition	Observation point					
	1	2	3	4	5	6
A	0.103	0.186	2.148	4.019	10.900	15.046
B	0.103	0.184	2.142	3.999	10.678	14.800
C	0.103	0.182	2.136	3.987	10.460	14.531
D	0.103	0.180	2.132	4.006	10.325	14.358



**Figure 9. Curves of concentration comparison (two months).**

method (linear programming) and numerical method. By their combined efforts the modular form is optimized and controlled. Namely, we take underground water variables (water level, discharge, concentration and so on) in differential equations as the decision variables, use difference method change them into linear algebraic equation groups and introduce them into linear programming model as the constraint conditions.

Now we perform numerical simulation of a real project. Assume that there are two pumping wells lying in some area, whose quantities of pumping water are 4940 m<sup>3</sup>/d and 4227 m<sup>3</sup>/d, respectively. Taking some observed well A near pumping wells as a new observed well and applying previous methods, we optimize and study adjusted project modes under different cases.

Let it be supposed that the maximum quantity of pumping water of each well is never more than 5000 m<sup>3</sup>/d during winter without any rain. Three cases are considered here to optimize the quantity of each well with adjusted computation. The first case is that the groundwater level of observed well doesn't decrease (Case 1). The second case is that the increase of the level is less than 0.1 m (Case 2). And the last case is that the increase of the level is more than 0.1 m (Case 3). Numerical data under three cases described above are illustrated in **Table 6**.

With three cases considered above, prediction for seawater intrusion problems is shown in **Table 7**, and the salt concentration of Case 1 is shown in **Figure 10**.

From the data in tables, it is easily seen that the second pumping well affects more heavily than the first one as for the level of observed wells. Thus, we can draw the following conclusions.

- 1) For the fixed pumping well and observed well, the

**Table 6. Adjusted mode of water saving project (m<sup>3</sup>/d).**

Quantity	Pumping well number		
	1	2	3
Case 1	5000	1840	6840
Case 2	5000	1620	6620
Case 3	5000	2050	7050

**Table 7. Changes of salt concentration in soil under different conditions (mg/L).**

Water head	Observation point					
	1-1	2-2	3-2	4-2	5-2	6-2
Case 1	3875	3043	1494	101	98	100
Case 2	3870	3042	1491	101	98	100
Case 3	3924	3056	1526	101	98	99

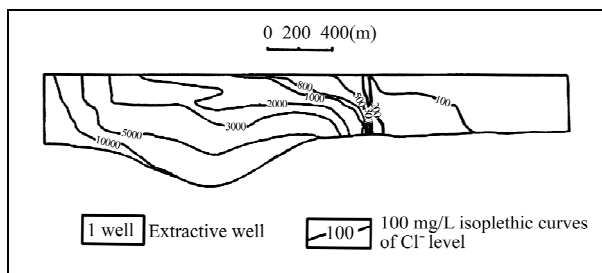


Figure 10. The salt concentration of Case 1.

first pumping well can work in the usual form while the second one should be strictly restricted by applying some water saving rules nearby.

2) Needs of the second pumping well should be firstly considered in Yellow River Diversion Project.

If the locations of pumping wells and observation points are different, the regulation modular forms are different too. With the establishment of ecological and environmental control projects, it is possible to get the timely and accurate observation data about seawater intrusion. Therefore, the established control model can do control model calculation for all projects in the entire region.

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