Analysis in Theory and Applications
Anal. Theory Appl., Vol. **41**, No. 2 (2025), pp. 111-139

DOI: 10.4208/ata.OA-2022-0024
June 2025

An Upwind Multistep Difference with Mixed Finite Volume Element Method for a Positive Semi-Definite Contamination Treatment Problem

Changfeng Li[1,2], Yirang Yuan[2,*] and Huailing Song[2]

[1] *School of Economics, Shandong University, Jinan, Shandong 250100, China*
[2] *Institute of Mathematics, Shandong University, Jinan, Shandong 250100, China*
[3] *College of Mathematics and Econometrics, Hunan University, Changsha, Hunan 410082, China*

Received 8 August 2022; Accepted (in revised version) 19 March 2025

Abstract. A positive semi-definite problem of three-dimensional incompressible contamination treatment from nuclear waste in porous media is discussed in this paper. The mathematical model is defined by a nonlinear initial-boundary system consisting of partial differential equations. Four important equations (an elliptic equation, two convection-diffusion equations and a heat conductor equation) determine the physical features. Considering the physical natures and computational efficiency, the authors introduce the conservative mixed finite volume element, upwind approximation and multistep difference to solve this system. The pressure and Darcy velocity are computed by a mixed finite volume element. The concentrations and temperature are solved by a combination of upwind approximation, multistep difference and mixed finite volume element. A multistep difference is used for approximating the partial derivative with respect to time. Mixed finite volume element and upwind differences are given for solving the convection-diffusions equations. Numerical dispersion and nonphysical oscillations could be eliminated, and the computational efficiency is improved by using a large time step. Furthermore, a conservative law is preserved and error estimates in L^2-norm is obtained. Finally, two numerical experiments are given to show the efficiency and possible applications.

Key Words: Positive semi-definite problem, upwind multistep difference with mixed finite volume element, local conservation, convergence analysis, numerical experiments.
AMS Subject Classifications: 65M15, 65N30, 65N12, 76S05

1 Introduction

An upwind multistep difference with mixed finite volume element (UMDMFVE) is proposed for a nuclear waste contamination disposal problem with positive semi-definite

*Corresponding author. *Email address:* `yryuan@sdu.edu.cn` (Y. Yuan), `cfli@sdu.edu.cn` (C. Li), `shling@hnu.edu.cn` (H. Song)

diffusion in porous media, and numerical analysis is shown in this paper. At present, nuclear waste is usually deposited in underground deep space. A challenging problem is how the diffusion is controlled and destructive disaster is avoided once natural calamities, such as earthquake or rock fracture, take place. Numerical methods are introduced for possibly simulating the true physical natures. Then, some positive suggestions possibly are put forward for contamination treatment. An incompressible positive semi-definite mathematical model is discussed [1–5]. The physical features are included as follows: the movement of flow (the pressure $p(X,t)$), the convection-diffusion displacement of brine (the concentration $\hat{c}$), the displacement of ith radionuclide trace contamination (the concentration $\{c_i\}$), and the heat conduction migration (the temperature $T(X,t)$).

Fluid:

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

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

where $p(X,t)$ and $\mathbf{u}=\mathbf{u}(X,t)$ are the fluid pressure and Darcy velocity, respectively. $q=q(X,t)$ is the production. $R_s'=R_s'(\hat{c})$ is a salt dissolution term of main contamination, and $\kappa(X)$ is the permeability of rock. $\mu(\hat{c})$ is the viscosity.

The concentration of brine (main contamination):

$$\phi\frac{\partial\hat{c}}{\partial t} + \mathbf{u}\cdot\nabla\hat{c} - \nabla\cdot(\mathbf{E}_c(\mathbf{u})\nabla\hat{c}) = f(\hat{c}), \quad X\in\Omega, \quad t\in J, \tag{1.2}$$

where ϕ is the porosity. $\mathbf{E}_c(\mathbf{u})$ is the diffusion tensor including the molecular diffusion and mechanical diffusion,

$$\begin{aligned}\mathbf{E}_c(\mathbf{u}) =&\phi d_m\mathbf{I} + d_l|\mathbf{u}|^\beta\begin{pmatrix}\hat{u}_x^2 & \hat{u}_x\hat{u}_y & \hat{u}_x\hat{u}_z\\ \hat{u}_x\hat{u}_y & \hat{u}_y^2 & \hat{u}_y\hat{u}_z\\ \hat{u}_x\hat{u}_z & \hat{u}_y\hat{u}_z & \hat{u}_z^2\end{pmatrix}\\ &+ d_t|\mathbf{u}|^\beta\begin{pmatrix}\hat{u}_y^2+\hat{u}_z^2 & -\hat{u}_x\hat{u}_y & -\hat{u}_x\hat{u}_z\\ -\hat{u}_x\hat{u}_y & \hat{u}_x^2+\hat{u}_z^2 & -\hat{u}_y\hat{u}_z\\ -\hat{u}_x\hat{u}_z & -\hat{u}_y\hat{u}_z & \hat{u}_x^2+\hat{u}_y^2\end{pmatrix}\\ =&D_m\mathbf{I} + D(\mathbf{u}).\end{aligned} \tag{1.3}$$

d_m is molecular diffusion and $D_m=\phi d_m$. $\mathbf{I}$ ia a 3×3 identity matrix. d_l and d_t the longitudinal diffusion and transverse coefficient, respectively. $\hat{u}_x,\hat{u}_y,\hat{u}_z$ are three direction cosines of Darcy velocity. Generally, take $\beta\geq 2$, and let

$$f(\hat{c}) = -\hat{c}\{[c_s\phi K_s f_s/(1+c_s)](1-\hat{c})\} - q_c - R_s.$$

The concentrations of radionuclide (trace contamination factors):

$$\begin{aligned}&\phi K_i\frac{\partial c_i}{\partial t} + \mathbf{u}\cdot\nabla c_i - \nabla\cdot(\mathbf{E}_c(\mathbf{u})\nabla c_i)\\ =&f_i(\hat{c},c_1,c_2,\cdots,c_{\hat{N}}), \quad X\in\Omega, \quad t\in J, \quad i=1,2,\cdots,\hat{N}.\end{aligned} \tag{1.4}$$