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

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

AMS subject classifications: 65M15, 65N30, 65N12, 76S05

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Key words: Compressible nuclear waste contamination in porous media, upwind mixed volume element-fractional step on a changing mesh, conservation of mass and energy, convergence analysis, numerical example.

1 Introduction

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

Fluid:

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

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

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

Heat:

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

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

The concentration of brine (main contamination):

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