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A new finite volume scheme preserving positivity for radionuclide transport calculations in radioactive waste repository

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ABSTRACT

In order to simulate a far field model used in geological radioactive waste repository, a new finite volume scheme preserving positivity on arbitrary convex polygonal meshes with second order accuracy is proposed in this paper. The model problem describes the coupled process of diffusion, convection and chemical reaction, in which the diffusion tensors are highly anisotropic and heterogeneous. The classic implicit and explicit schemes are used in the temporal discretization. The discretization of diffusive flux in Sheng and Yuan (2016) is utilized, and the discretization of convective flux is based on a new corrected upwind scheme that depends on some available informations of diffusive flux. The resulting scheme is positivity-preserving and locally conservative, and has only cell-centered unknowns. Numerical results are presented to show that the performance of our positivity-preserving scheme for the numerical simulation of radionuclide transport problem.

1. Introduction

The exploitation and utilization of nuclear power produce high level radioactive wastes. A key issue is how to deal with these wastes safely and efficiently. One method is transmutation, although the most nuclides would be separated and modified to be less harmful, the technology is not mature. Hence, several nuclear countries choose geological disposal to handle the radioactive waste, i.e., geological radioactive waste repository system. The nuclear waste are placed into containers, and the containers are placed into a depth of several hundreds meters, which is well below groundwater surface. Then, the groundwater maybe access to the containers. Once a container leaks, groundwater can transport radionuclides for a long distance. So it is essentially necessary to provide an efficient estimate for safety assessment to the high-level radioactive waste repository system.

In [13], it is pointed out that some particular features must be considered for numerically simulating the radioactive waste repository. First, in consideration of the repository components of cylindrical shape, such as waste canisters and so on, an unstructured mesh must be used. Second, geological formations and materials are strongly heterogeneous. For example, the host rock consists of a very low permeability material where the flow is very slow and the transport is diffusion-dominated, then, in another layer such as aquifers, the water flow is faster and the transport is convection-dominated. Third, the dispersivity inside the aquifer is highly anisotropic. Hence, how to construct an efficient and accurate scheme for solving such kinds of model is very important.

In general, a scheme should be consistent, stable and maintain some qualitative properties on the discrete level, such as local conservation and maximum principle. From the numerical point of view, it is difficult to construct a scheme to satisfy the discrete maximum principle on distorted meshes for convection-diffusion-reaction equation, especially in the case that the magnitude of convection velocity is much larger than the diffusive coefficient. So, a weaker version of maximum principle is considered, i.e., positivity-preserving, which is one of the key points for discrete schemes.

For the approximation of diffusive term, in order to preserve positivity, some restrictive conditions on diffusive coefficients and meshes are imposed [11,21,24], and some preprocessing or postprocessing methods are proposed [1,8,32]. In recent years, some nonlinear schemes without these restrictive conditions have been proposed [10,18,19,25,27,29–31,35].

For the approximation of convective term, the gradient reconstruction [4,5,12,15,20,22,33,34] is one of the most popular method, where the convective flux can be approximated by the upwind approach [2] and controlled by different slope limiting techniques [5,6,9,17]. Bertolazzi [4] proposed a MUSCL-like

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cell-centered finite volume method, where the discretization of advective fluxes is based on a least-square reconstruction of the vertex values from cell averages. Lipnikov [20] proposed a new slope limiting technique based on a specially minimal nonlinear correction, which follows the ideas of the monotonic upstream-centered scheme for conservation laws (MUSCL). Then, in [33,36], the limiting technique is used to avoid nonphysical oscillation.

In this work, we introduce a new gradient reconstruction method and construct a finite volume scheme preserving positivity with second order accuracy for the steady convection-diffusion equation on arbitrary convex polygonal meshes. The discretization of diffusive flux in [31] is utilized. We focus on the discretization of convective flux, since there exists already information in the discretization of diffusive flux, a new corrected method is proposed to improve the accuracy. Our method can assure the positivity and improve the accuracy. It is different with some existing schemes such as [20,33,36]. Moreover, our method is very efficient for some large deformed meshes, such as Kershaw mesh [14], which is a challenging problem for the finite volume scheme. Then, we extend it to the unsteady convection-diffusion-reaction equation, and prove that the scheme can preserve positivity. At last, two applications of radioactive waste repository are tested to show the effectiveness of our scheme, we use the nine point scheme [28] and our positivity-preserving scheme with the classic explicit and implicit discretization. Numerical results show that our fully implicit positivity-preserving scheme is more efficient.

The article is organized as follows. The model problem is described and some notations are introduced in Section 2. The main idea of construction for 1D steady convection-diffusion equation is given in Section 3. The discretization of diffusive and convection flux is given in Section 4. In Section 5, we show that our scheme can preserve the positivity, and give the in detail. In Section 6, two numerical tests are exhibited to illustrate the features of our scheme. At last, some conclusions are given in Section 7.

2. The model problem

2.1. Radionuclide transport problem

We consider the radionuclide transport equations [13,23], and more specifically the transport of the ^{129}I. It escapes from a waste repository vault into the water and its concentration is given by the following unsteady convection-diffusion-reaction equation:

$$\omega\frac{\partial C}{\partial t}-\nabla\cdot(\overline{D}\nabla C-\vec{U}C)+\omega\lambda C=0 \quad \text{in } \Omega\times(0,T), \tag{1}$$

where C is the solute concentration, $\lambda = log2/T_e$ with T_e being the half life of the element, ω is the effective porosity, $\overline{D} = D_e + \bar{\alpha}(\alpha_T, \alpha_L, \vec{U})$ is the diffusion tensor where D_e is the effective diffusion tensor and $\bar{\alpha}$ is the dispersive tensor, where $\alpha_T,\ \alpha_L$ is transverse and longitudinal dispersivity, respectively.

In the Eq. (1), Darcy's velocity $\vec{U}$ is given by Darcy's law:

$$\begin{cases}\nabla\vec{U} &= 0,\\ \vec{U} &= -\overline{K}\nabla H,\end{cases} \tag{2}$$

where $\overline{K}$ is the permeability tensor, and H is the head.

2.2. Mathematical model

Now, we consider the following unsteady convection-diffusion-reaction equation for unknown function u:

$$b\frac{\partial u}{\partial t}-\nabla\cdot(\kappa\nabla u-vu)+cu=f, \quad \text{in } \Omega\times(0,T), \tag{3}$$

$$u=g, \quad \text{on } \partial\Omega\times(0,T), \tag{4}$$

$$u=u_0, \quad \text{in } \Omega\times\{0\}, \tag{5}$$

where Ω is a bounded polygonal domain in R^2 with boundary $\partial\Omega$, $v = v(\mathbf{x}, t)$ is a velocity vector field and $\kappa = \kappa(\mathbf{x}, t)$ is a diffusion tensor, $b > 0$ is constant. Assume that the functions $c = c(\mathbf{x}, t), f = f(\mathbf{x}, t), g = g(\mathbf{x}, t)$ and v satisfy the following constraints:

$$\nabla\cdot v\geqslant 0,\ \ v\in C^1(\bar{\Omega})^2, \tag{6}$$

$$c\in L^\infty(\Omega\times(0,T)), c\geqslant 0, \tag{7}$$

$$f\in L^\infty((0,T);L^2(\Omega)), \tag{8}$$

$$g\in L^\infty((0,T);H^{1/2}(\partial\Omega)\cap C(\partial\Omega)), \tag{9}$$

and there are two positive constants λ_1 and λ_2 such that

$$\lambda_1|\xi|^2\leqslant\kappa\xi\cdot\xi\leqslant\lambda_2|\xi|^2, \forall\xi\in R^2.$$

The assumption $\nabla\cdot v \geqslant 0$ is not a necessary condition in Eq. (6), so it can be neglected. We only need $v \in C^1(\bar{\Omega})^2$. Meanwhile, $c \geqslant 0$ is also not a necessary condition in assumption (7), too, it can be weakened to $c \geqslant -c_0$ (c_0 is a positive constant). The reason that the condition is strengthened into the present form is to give a simple proof for the positivity-preserving. When the conditions (6) and (7) are weakened, in order to guarantee the positivity of the scheme, a restriction on the time step (Δt) must be introduced, i.e., $(c_0 + \|\nabla\cdot v\|_\infty)\Delta t < 1$.

3. The 1D problem

We first describe the basic idea of finite volume scheme preserving positivity for 1D steady convection-diffusion equation briefly, that is

$$-\kappa\frac{\partial^2 u}{\partial x^2}+b\frac{\partial u}{\partial x}=f, \quad \text{in } \Omega, \tag{10}$$

$$u=g, \quad \text{on } \partial\Omega, \tag{11}$$

where Ω is a bounded domain $[l_1, l_2]$ with boundary $\partial\Omega, b = b(x)$ is a velocity, $\kappa = \kappa(x)$ is a diffusive coefficient and $f(x)$ is the source.

Divide the interval $[l_1, l_2]$ with $I_i := [x_{i-1/2}, x_{i+1/2}],\ i = 1, 2, \ldots, N$, where $x_{1/2} = l_1, x_{N+1/2} = l_2$. See Fig. 1. We define $h = (l_2 - l_1)/(N - 1)$ and integrate (10) at each interval I_i to obtain

$$\int_{x_{i-1/2}}^{x_{i+1/2}}\left(-\kappa\frac{\partial^2 u}{\partial x^2}+b\frac{\partial u}{\partial x}\right)dx=\int_{x_{i-1/2}}^{x_{i+1/2}}f(x)dx. \tag{12}$$

With Green's formula, we obtain

$$\mathcal{F}_{i,i-1/2}+\mathcal{F}_{i,i+1/2}+\mathcal{G}_{i,i-1/2}+\mathcal{G}_{i,i-1/2}=\int_{x_{i-1/2}}^{x_{i+1/2}}f(x)dx, \tag{13}$$

where $\mathcal{F}_{P,Q}, \mathcal{G}_{P,Q}$ are the continuous diffusive and convective flux at the point Q of cell P, respectively. Actually, the expression of diffusive flux can be written as the following form, that is

$$\mathcal{F}_{i,i-1/2}+\mathcal{F}_{i,i+1/2}=-\kappa_i\frac{u_{i-1}-2u_i+u_{i+1}}{h}+O(h^2). \tag{14}$$

It satisfies the discrete maximum principle clearly.

We focus on the discretization of convective flux, where

$$\mathcal{G}_{i,i-1/2}=-b(x_{i-1/2})u(x_{i-1/2})=-\bar{u}_{i-1/2}(b^+_{i-1/2}-b^-_{i-1/2})+O(h^2), \tag{15}$$

$$\mathcal{G}_{i,i+1/2}=\quad b(x_{i+1/2})u(x_{i+1/2})=\bar{u}_{i+1/2}(b^+_{i+1/2}-b^-_{i+1/2})+O(h^2). \tag{16}$$

and

$$b^+_j=\frac{|b_j|+b_j}{2}, \quad b^-_j=\frac{|b_j|-b_j}{2}, \quad (j=i-1/2, i+1/2).$$