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An Error Estimate of a Modified Method of Characteristics Modeling Advective-Diffusive Transport in Randomly Heterogeneous Porous Media

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Abstract. We analyze a stochastic modified method of characteristics (MMOC) modeling advective-diffusive transport in randomly heterogeneous porous media. Under the log-normal assumption of the porous media and the finite-dimensional noise assumption that leads to unbounded diffusivity, we prove an optimal-order error estimate for the stochastic MMOC scheme. Numerical experiments are presented to substantiate the numerical analysis.

AMS subject classifications: 65M25, 65M60, 65Z05, 76M10

Key words: Uncertainty quantification, MMOC, advective-diffusive transport.

1 Introduction

The objective in many applications such as remediation of contaminated aquifers, miscible displacement in enhanced oil recovery, and CO_2 sequestration is to accurately predict the moving steep fronts of the concentration of the solute or injected solvent to optimize the remediation or recovery process [4, 11, 20, 26, 35]. Ideally, with the given information on the media (e.g., permeability and porosity) and fluid (e.g., the pressure and the concentration of the solute or solvent at the injection wells or sources of the contaminations and at the production wells or monitoring wells), one should be able to determine the movement of the solute or solvent. However, many very difficult mathematical and numerical obstacles occur. The mapping from the given data to the concentration of the solute/solvent is a strongly coupled, nonlinear and dynamic process, in which the

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transport of the solute/solvent depends heavily on the Darcy velocity of the fluid while the viscosity of the fluid may in turn depend on the concentration of solvent. Furthermore, information on subsurface porous media is very limited and available only near the injection and production (or monitoring) wells. Due to the high spatial variability of geological properties of porous media and the scarcity of available data, the hydrological parameters describing macroscopic properties of porous media, such as the intrinsic permeability and porosity, cannot be accurately characterized in detail and are often modeled as spatially correlated random fields [7,16,45]. These parameters strongly affect the transport processes, thus rendering the transport processes uncertain and making the flow and transport equations stochastic. In summary, the mathematical models lead to strongly coupled nonlinear systems of time-dependent advection-diffusion equations that present moving steep fronts, where complex physical and chemical phenomena take place that need to be resolved accurately in applications [4,11,20,27].

Upwind methods are widely used in industrial applications to stabilize the numerical approximations to these systems in large-scale simulators, but they tend to produce numerical solutions with excessive numerical diffusion and spurious grid orientation effects [11,33]. On the other hand, Eulerian-Lagrangian methods [2,8,9,12,14,23,31–33,37,39] combine the advection term with the capacity term in the transport equation and carry out the temporal discretization through a characteristic tracking. They symmetrize the transport equation and yield a symmetric and positive definite linear algebraic system. Moreover, they naturally cancel out the majority of the temporal error in the transport equation, which most Eulerian methods attempt to reduce via different techniques, by the spatial error from the advection term. Therefore, Eulerian-Lagrangian methods generate accurate numerical solutions even if large time steps and coarse spatial grids are used, and are very competitive with many numerical methods [33, 34]. Furthermore, they eliminate the excessive numerical diffusion and grid orientation effect present in upstream-weighted, large-scale numerical simulators in industrial production [11,36].

In this paper we develop a stochastic MMOC method, an MMOC-based stochastic Galerkin method [13,44,46], for a time-dependent advection-diffusion equation modeling solute transport in randomly heterogeneous porous media. We follow the treatment in [3,18,28,30,42,43,45] to make a physically relevant assumption that the diffusivity coefficient is log-normal, which is unbounded and violates the conventional assumption that the diffusivity has uniform lower and upper bounds, cf. e.g., [3, Equation 5.2] and [5, Equation 1.1], that is crucial in the corresponding analysis. Furthermore, the spatial eigenfunctions and the random variables are coupled in the Karhunen-Loéve expansion in the random diffusivity coefficient. Thus the developed numerical analysis frameworks for the MMOC to deterministic problems (cf. e.g., [8,9]), which are based on the boundedness of the diffusivity coefficients, do not directly apply. Besides, due to the dependence of the diffusivity coefficient on stochastic variables, which will change their original joint density function, some estimates of the projection in parametric space are affected and require unconventional treatments (cf. Lemma 5.2).

The rest of the paper is organized as follows. In Section 2 we formulate the mathematical model. In Section 3 we present preliminaries to be used subsequently. In Section 4 we present the stochastic MMOC scheme. In Section 5 we prove an optimal-order error estimate of the stochastic MMOC scheme. In Section 6 we carry out numerical experiments to substantiate the numerical analysis. We present concluding remarks in Section 7.

2 Problem formulation

Let $(\Omega,\mathcal{F},\mu)$ be a complete probability space, with Ω being the sample space, $\mathcal{F}$ a σ-algebra of subsets of Ω, and μ a probability measure. Then $g=g(\boldsymbol{x},t,\omega)$ represents a quantity of interest with randomness in the porous medium, where $\boldsymbol{x}\in G$ with $G\subset\mathbb{R}^d$ $(1\leq d\leq 3)$ being the spatial bounded polyhedron domain with smooth boundary, $t\in[0,T]$ for some $T>0$, and ω is the sample point in the sample space Ω.

Let c be the concentration of the solute in the fluid flow. We consider the following advection-diffusion equation with randomness modeling the solute transport process in a porous medium reservoir G over a time period of $[0,T]$ [4,11]

$$\phi\frac{\partial c(\boldsymbol{x},t,\omega)}{\partial t}+\boldsymbol{u}(\boldsymbol{x},t)\cdot\nabla c(\boldsymbol{x},t,\omega)-\nabla\cdot(D(\boldsymbol{x},\omega)\nabla c(\boldsymbol{x},t,\omega))=f(\boldsymbol{x},t,\omega). \tag{2.1}$$

Here $0<\phi_0\leq\phi(\boldsymbol{x})<1$ for some $\phi_0>0$ is the permeability, $\boldsymbol{u}$ represents the Darcy velocity of the fluid, D stands for the diffusivity coefficient, f refers to the source or sink term, and we assume that the transport equation is closed by an initial value $c_0(\boldsymbol{x})$ and a periodic boundary condition or the solution is compactly supported inside the domain G [8,9,11].

We next specify the form of the diffusivity coefficient D. Let $Y(\boldsymbol{x},\omega)$ be a second-order continuous stationary random process with multivariate Gaussian distribution

$$\mathbb{E}[|Y(\boldsymbol{x},\omega)|^2]<+\infty \quad \text{and} \quad \lim_{\boldsymbol{x}_2\to\boldsymbol{x}_1}\mathbb{E}[|Y(\boldsymbol{x}_2,\omega)-Y(\boldsymbol{x}_1,\omega)|^2]=0.$$

Then $Y(\boldsymbol{x},\omega)$ can be expanded in terms of the Karhunen-Loéve expansion [18]

$$Y(\boldsymbol{x},\omega)=\bar{Y}(\boldsymbol{x})+\sum_{i=1}^{\infty}\sqrt{\lambda_i}\zeta_i(\omega)\psi_i(\boldsymbol{x}), \tag{2.2}$$

where $\bar{Y}(\boldsymbol{x})$ denotes the mean of $Y(\boldsymbol{x},\omega)$, the modulus of which is assumed to be bounded by a positive constant $C(\bar{Y})$. $\{\lambda_i\}_{i=1}^{\infty}$ and $\{\psi_i(\boldsymbol{x})\}_{i=1}^{\infty}$ are the corresponding sets of eigenvalues and orthonormal eigenfunctions of the following eigenvalue problems

$$\int_G C_Y(\boldsymbol{x_1},\boldsymbol{x_2})\psi_i(\boldsymbol{x_2})d\boldsymbol{x_2}=\lambda_i\psi_i(\boldsymbol{x_1}), \quad \boldsymbol{x_1}\in G, \tag{2.3}$$

where $C_Y(\boldsymbol{x_1},\boldsymbol{x_2})=cov(Y(\boldsymbol{x_1},\cdot),Y(\boldsymbol{x_2},\cdot))$ is the symmetric and positive-definite covariance kernel. $\{\zeta_i(\omega)\}_{i=1}^{\infty}$ is the set of mutually uncorrelated random variables with zero mean and unit variances given by

$$\zeta_i(\omega)=\frac{1}{\sqrt{\lambda_i}}\int_G (Y(\boldsymbol{x},\omega)-\bar{Y}(\boldsymbol{x}))\psi_i(\boldsymbol{x})d\boldsymbol{x}, \quad 1\leq i<\infty. \tag{2.4}$$

To ensure the convergence of the series in (2.2), we follow [19, Equation 6] to assume that $\sum_{i=1}^{\infty}\|\sqrt{\lambda_i}\psi_i(\boldsymbol{x})\|_{L^\infty(G)}<\infty$. Under this assumption, there exists a constant $Q_0>0$ such that

$$\max_{1\leq i\leq\infty}\|\sqrt{\lambda_i}\psi_i(\boldsymbol{x})\|_{L^\infty(G)}\leq Q_0. \tag{2.5}$$

Indeed, under some smoothness assumptions of C_Y, $\|\sqrt{\lambda_i}\psi_i(\boldsymbol{x})\|_{L^\infty(G)}$ decays very fast with respect to i, see e.g. [5, Equation 2.18]. Consequently, (2.5) is satisfied and the Karhunen-Loéve expansion (2.2) is usually truncated to a finite number of terms in real applications for some $M>0$ [3], which is physically relevant as any measurement can only keep tracking the fine scale information to certain limit [3,7,26,45]

$$Y_M(\boldsymbol{x};\omega)=\bar{Y}(\boldsymbol{x})+\sum_{i=1}^{M}\sqrt{\lambda_i}\zeta_i(\omega)\psi_i(\boldsymbol{x})=\bar{Y}(\boldsymbol{x})+Y_c(\boldsymbol{x};\boldsymbol{\zeta}), \tag{2.6}$$

with $Y_c(\boldsymbol{x};\boldsymbol{\zeta})=\sum_{i=1}^{M}\sqrt{\lambda_i}\zeta_i(\omega)\psi_i(\boldsymbol{x})$ being a mean zero random function such that the corresponding optimal mean-square truncation error

$$\int_G \mathbb{E}\big[|Y(\boldsymbol{x};\omega)-Y_M(\boldsymbol{x};\omega)|^2\big]d\boldsymbol{x}=\sum_{i=M+1}^{\infty}\lambda_i, \tag{2.7}$$

is sufficiently small, which depends on the decay rate of the eigenvalues $\{\lambda_i\}_{i=1}^{\infty}$ that in turn depends on the regularity of the correlation function and its correlation length.

Consequently, we follow [3,18,42,43,45] to assume a log-normal diffusion coefficient D depending on finitely many random variables in (2.1), the form of which could be found in, e.g., [17, Equation 2.6] and [19, Equation 8]

$$D(\boldsymbol{x},\omega)=\rho_0(\boldsymbol{x})+\rho_1(\boldsymbol{x})e^{Y_M(\boldsymbol{x},\omega)}, \tag{2.8}$$

where $0<\rho_*\leq\rho_0\leq\rho_{**}<\infty$ and $0\leq\rho_1\leq\rho_{**}$ for some positive constants $0<\rho_*\leq\rho_{**}$ represent the molecule diffusion and mechanical dispersion coefficient, respectively. Since Y_M is normal, $D(\boldsymbol{x},\omega)$ may be unbounded, which contradicts the conventional assumption that D has the positive lower and upper bounds. We follow [19] to denote the coordinate of ζ_i by y_i for $1\leq i\leq M$ and define $\boldsymbol{y}=(y_1,\cdots,y_M)$. Then the diffusivity coefficient D in (2.8) may also be written as [19, Equation 8]

$$D(\boldsymbol{x},\boldsymbol{y})=\rho_0(\boldsymbol{x})+\rho_1(\boldsymbol{x})\exp\Big(\bar{Y}(\boldsymbol{x})+\sum_{i=1}^{M}\sqrt{\lambda_i}y_i\psi_i(\boldsymbol{x})\Big). \tag{2.9}$$

In the rest of this paper we follow the convention to assume that the input random field can be decomposed in the form of (2.6) [3], either because they can be approximated by, e.g., a truncated Karhunen-Loéve expansion or because they can often be explicitly defined in terms of a finite number of random variables like (2.6).

3 Preliminaries

We introduce notations and projections frequently used in the rest of the paper.

3.1 Spaces and norms

Let $L^p(G)$ with $1\le p\le\infty$ be the spaces of pth Lebesgue integrable functions on G and $H^m(G)$ be the Hilbert spaces of functions with derivatives of order m in $L^2(G)$. Let $H_0^m(G)$ be the completion of $C_0^\infty(G)$, the space of infinitely differentiable functions with compact support in G, in $H^m(G)$. All the spaces are equipped with the standard norms [1].

For any Banach space X, we introduce Sobolev spaces involving time [10]

$$W_p^k(t_1,t_2;X):=\Big\{g:\Big\|\frac{\partial^l g}{\partial t^l}(\cdot,t)\Big\|_X\in L^p(t_1,t_2),\ 0\le l\le k,\ 1\le p\le\infty\Big\},$$

$$\|g\|_{W_p^k(t_1,t_2;X)}:=\begin{cases}\displaystyle\Big(\sum_{l=0}^k\int_{t_1}^{t_2}\Big\|\frac{\partial^l g}{\partial t^l}(\cdot,t)\Big\|_X^p dt\Big)^{1/p}, & 1\le p<\infty,\\ \displaystyle\max_{0\le l\le k}\operatorname*{ess\ sup}_{t\in(t_1,t_2)}\Big\|\frac{\partial^l g}{\partial t^l}(\cdot,t)\Big\|_X, & p=\infty.\end{cases}$$

For a positive integer M, the weighted L^p space on $\mathbb{R}^M$ for $1\le p<\infty$ weighted by $\pi(\boldsymbol{y})\ge 0$ with $\boldsymbol{y}=(y_1,\cdots,y_M)\in\mathbb{R}^M$ is defined by $L_\pi^p(\mathbb{R}^M)=\{g:g$ is measurable and $\|g\|_{L_\pi^p(\mathbb{R}^M)}<\infty\}$, subject to the norm $\|g\|_{L_\pi^p(\mathbb{R})}:=\big(\int_{\mathbb{R}^M}|g(\boldsymbol{y})|^p\pi(\boldsymbol{y})d\boldsymbol{y}\big)^{1/p}$. The weighted Sobolev space $W_{p,\pi}^k(\mathbb{R}^M)$ consists of functions with derivatives up to order k in $L_\pi^p(\mathbb{R}^M)$ and endowed with the norm

$$\|g\|_{W_{p,\pi}^k(\mathbb{R}^M)}:=\bigg(\sum_{|\boldsymbol{l}|=0}^k\Big\|\frac{d^{|\boldsymbol{l}|}g}{d\boldsymbol{y}^{\boldsymbol{l}}}\Big\|_{L_\pi^p(\mathbb{R}^M)}^p\bigg)^{\frac{1}{p}},\quad |\boldsymbol{l}|:=\sum_{j=1}^M l_j,\quad d\boldsymbol{y}^{\boldsymbol{l}}:=dy_1^{l_1}\cdots dy_M^{l_M}.$$

In particular, we denote $W_{2,\pi}^k(\mathbb{R}^M)$ by $H_\pi^k(\mathbb{R}^M)$ for simplicity.

For the convenience of the error estimates, we introduce discrete norms based on the temporal partition $\{t_n\}_{n=0}^{N_t}$ of $[0,T]$ where $t_n:=n\Delta t$ with $\Delta t=T/N_t$ for some integer $N_t>0$

$$\|g\|_{\hat{L}^\infty(0,t_N;X)}:=\max_{0\le n\le N}\|g(\cdot,t_n)\|_X,\quad \|g\|_{\hat{L}^2(0,t_N;X)}:=\Big(\sum_{n=0}^N\|g(\cdot,t_n)\|_X^2\Delta t\Big)^{1/2}.$$

We further define the inner product

$$\langle g_1,g_2\rangle_{L^2(G;L_\pi^2(\mathbb{R}^M))}:=\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\int_G g_1(\boldsymbol{x},\boldsymbol{y})g_2(\boldsymbol{x},\boldsymbol{y})d\boldsymbol{x}d\boldsymbol{y}, \tag{3.1}$$

for $g_1,\ g_2\in L^2(G)\times L_\pi^2(\mathbb{R}^M)$ and

$$\|g\|_{L^2(G;L_\pi^2(\mathbb{R}^M))}:=\langle g,g\rangle_{L^2(G;L_\pi^2(\mathbb{R}^M))}^{1/2}. \tag{3.2}$$

In the rest of the paper we set $\pi(\boldsymbol{y}) := e^{-y_1^2/2}\times\cdots\times e^{-y_M^2/2}/(\sqrt{2\pi})^M$ and denote the generic constant by Q that may assume different values at different occurrences.

3.2 L^2 projection from $L^2_\pi(\mathbb{R}^M)$ to $P_N(\mathbb{R}^M)$

A natural choice of the finite-dimensional subspace $P_N(\mathbb{R}^M)$ of $L^2_\pi(\mathbb{R}^M)$ is

$$P_N(\mathbb{R}^M) := \left\{ v : \mathbb{R}^M \to \mathbb{R} \,\middle|\, v = \sum_{i_1=0}^{N}\cdots\sum_{i_M=0}^{N} c_{i_1,\cdots,i_M} H_{i_1}(y_1)\cdots H_{i_M}(y_M) \right\}, \tag{3.3}$$

where $H_j(z)$ refers to the j-th Hermite polynomial defined by

$$H_0(z)=1,\quad H_1(z)=z,\quad H_{j+1}(z)=zH_j(z)-jH_{j-1}(z),\quad j\geq 2,$$

associated with the weight function $e^{-z^2/2}$ [25,29].

Define the weighted L^2 projection $\mathcal{T}: L^2_\pi(\mathbb{R}^M)\to P_N(\mathbb{R}^M)$ by

$$\int_{\mathbb{R}^M} (g(\boldsymbol{y})-\mathcal{T}g(\boldsymbol{y}))v(\boldsymbol{y})\pi(\boldsymbol{y})d\boldsymbol{y}=0,\quad \forall v\in P_N(\mathbb{R}^M). \tag{3.4}$$

For the one-dimensional case, the estimate of $g-\mathcal{T}g$ holds for $r\geq 0$ [29]

$$\|g-\mathcal{T}g\|_{L^2_{\hat\pi}(\mathbb{R})} \leq QN^{-\frac{r}{2}}\|g\|_{H^r_{\hat\pi}(\mathbb{R})},\quad \forall g\in H^r_\pi(\mathbb{R}),\quad \hat\pi(z)=e^{-z^2/2}/\sqrt{2\pi}. \tag{3.5}$$

To bound the projection error for the high dimensional case, we define the identity operator I and the one-dimensional analogue $\mathcal{T}_i$ of $\mathcal{T}$ on the ith direction for $1\leq i\leq M$. Then we apply the following relation

$$\begin{aligned} g-\mathcal{T}g &= g-\mathcal{T}_M\mathcal{T}_{M-1}\cdots\mathcal{T}_1 g \\ &= (I-\mathcal{T}_1)g+\mathcal{T}_1(I-\mathcal{T}_2)g+\cdots+\mathcal{T}_1\mathcal{T}_2\cdots\mathcal{T}_{M-1}(I-\mathcal{T}_M)g, \end{aligned}$$

together with (3.5) and the boundedness of the projection operator $\mathcal{T}_i$ to obtain

$$\|g-\mathcal{T}g\|_{L^2_\pi(\mathbb{R}^M)} \leq \sum_{i=1}^{M}\|(I-\mathcal{T}_i)g\|_{L^2_\pi(\mathbb{R}^M)} \leq QN^{-\frac{r}{2}}\|g\|_{H^r_\pi(\mathbb{R}^M)}. \tag{3.6}$$

We further note that $\mathcal{T}$ and ∇ are commutative, i.e.,

$$\begin{aligned} \nabla\mathcal{T}g &= \nabla\sum_{i_1=0}^{N}\cdots\sum_{i_M=0}^{N}\frac{\int_{\mathbb{R}^M}\pi(\boldsymbol{y})g(\boldsymbol{x},\boldsymbol{y})H_{i_1}(y_1)\cdots H_{i_M}(y_M)d\boldsymbol{y}}{\|H_{i_1}\|^2_{L^2_{\hat\pi}}\cdots\|H_{i_M}\|^2_{L^2_{\hat\pi}}}H_{i_1}(y_1)\cdots H_{i_M}(y_M) \\ &= \sum_{i_1=0}^{N}\cdots\sum_{i_M=0}^{N}\frac{\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\nabla g(\boldsymbol{x},\boldsymbol{y})H_{i_1}(y_1)\cdots H_{i_M}(y_M)d\boldsymbol{y}}{\|H_{i_1}\|^2_{L^2_{\hat\pi}}\cdots\|H_{i_M}\|^2_{L^2_{\hat\pi}}}H_{i_1}(y_1)\cdots H_{i_M}(y_M)=\mathcal{T}\nabla g. \end{aligned}$$

Remark 3.1. A more practical choice of P_N is the so-called sparse polynomial space, in which the sum of the orders of polynomials in all directions is up to N

$$\left\{ v: \mathbb{R}^M \to \mathbb{R} \,\middle|\, v = \sum_{|\boldsymbol{i}|=0}^{N} c_{i_1,\cdots,i_M} H_{i_1}(y_1)\cdots H_{i_M}(y_M) \right\}. \tag{3.7}$$

For a fixed N, the degree of freedom of the sparse polynomial space is much smaller than that of the full polynomial space (3.3), which is known as the "curse of dimensionality" that requires costly computations for large N. Furthermore, both (3.3) and (3.7) have similar approximation properties [25]. For this reason, we apply (3.3) in the subsequent analysis and all results can be directly extended to the case of using (3.7). In numerical experiments, we apply the sparse polynomial space (3.7) to reduce the computational costs.

3.3 Elliptic projection from $H_0^1(G)$ to $S_h(G)$

We define a quasi-uniform partition $\cup G_e$ of G with the maximal diameter h among all elements under the Euclidean norm $\|\cdot\|_{Euc}$ defined by $h := \max_{G_e\subset G} \max_{\boldsymbol{x}_1,\boldsymbol{x}_2\in G_e} \|\boldsymbol{x}_2 - \boldsymbol{x}_1\|_{Euc}$, and let $S_h(G)$ be the space of piecewise linear functions on this partition. For any fixed $\boldsymbol{y}\in\mathbb{R}^M$, standard elliptic projection $\mathcal{E}: H_0^1(G)\to S_h(G)$ is defined by

$$a(g-\mathcal{E}g, v_h) := \int_G D(\boldsymbol{x},\boldsymbol{y})\nabla(g-\mathcal{E}g)\nabla v_h \, d\boldsymbol{x} = 0, \quad \forall v_h \in S_h(G). \tag{3.8}$$

We employ (3.8) to obtain

$$\begin{aligned} \|D^{1/2}\nabla(\mathcal{E}g-g)\|^2_{L^2(G)} &= a(\mathcal{E}g-g, \mathcal{E}g-g) = a(\mathcal{E}g-g, v_h-g) \\ &\le \|D^{1/2}\nabla(\mathcal{E}g-g)\|_{L^2(G)} \cdot \|D^{1/2}\nabla(v_h-g)\|_{L^2(G)}, \quad \forall v_h\in S_h(G), \end{aligned}$$

which, together with (2.8) and the continuity of $\psi_i(\boldsymbol{x})$ (which follows from the continuity of C_Y and [21, Theorem 3.2.5]), yields

$$\begin{aligned} \sqrt{\rho_*}\|\nabla(\mathcal{E}g-g)\|_{L^2(G)} &\le \|D^{1/2}\nabla(\mathcal{E}g-g)\|_{L^2(G)} \\ &\le \inf_{\forall v_h\in S_h(G)} \|D^{1/2}\nabla(v_h-g)\|_{L^2(G)} \\ &\le \big(\rho(\boldsymbol{y})\big)^{1/2} \inf_{\forall v_h\in S_h(G)} \|\nabla(v_h-g)\|_{L^2(G)} \\ &\le Q\big(\rho(\boldsymbol{y})\big)^{1/2} h\|g\|_{H^2(G)}, \end{aligned} \tag{3.9}$$

where Q is a positive constant depending on d and the mesh parameters (cf. [6, Theorem 4.4.20]), and

$$\rho(\boldsymbol{y}) := \rho_{**} + \rho_{**} e^{C(\bar{Y})} \exp\Big(\sum_{i=1}^{M} |y_i| Q_0\Big), \tag{3.10}$$

where Q_0 is given by (2.5) and $\bar{Y}$ is defined in (2.6). Then a standard duality argument yields [6]

$$\|\mathcal{E}g-g\|_{L^2(G)} \le Q\rho(\boldsymbol{y})h^2\|g\|_{H^2(G)}. \tag{3.11}$$

Furthermore, selecting $v=\mathcal{E}g$ in (3.8) leads to the stability estimate of $\mathcal{E}g$

$$\|\nabla\mathcal{E}g\|_{L^2(G)} \le Q(\rho(\boldsymbol{y}))^{1/2}\|\nabla g\|_{L^2(G)}. \tag{3.12}$$

Define

$$\pi_*(\boldsymbol{y}):=\pi(\boldsymbol{y})\rho(\boldsymbol{y}), \tag{3.13}$$

and we integrate both sides of (3.9) on $\mathbb{R}^M$ to obtain for $g\in L^2_{\pi_*}(\mathbb{R}^M;H^2(G))$

$$\|\nabla(\mathcal{E}g-g)\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))} \le Qh^2\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\rho(\boldsymbol{y})\|g\|^2_{H^2(G)}d\boldsymbol{y} \le Qh^2\|g\|^2_{L^2_{\pi_*}(\mathbb{R}^M;H^2(G))}. \tag{3.14}$$

A similar operation for (3.11) with $\pi_{**}(\boldsymbol{y}):=\pi(\boldsymbol{y})\rho^2(\boldsymbol{y})$ yields for $g\in L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G))$

$$\|\mathcal{E}g-g\|_{L^2(G;L^2_\pi(\mathbb{R}^M))} \le Qh^2\|g\|_{L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G))}. \tag{3.15}$$

4 A stochastic MMOC

We first present the MMOC for the deterministic transport equation

$$\phi\frac{\partial c(\boldsymbol{x},t)}{\partial t}+\boldsymbol{u}(\boldsymbol{x},t)\cdot\nabla c(\boldsymbol{x},t)-\nabla\cdot(D(\boldsymbol{x})\nabla c(\boldsymbol{x},t))=f(\boldsymbol{x},t). \tag{4.1}$$

Denote τ the unit vector in the direction of $(\boldsymbol{u},\phi)$ in $G\times[0,T]$ and $\boldsymbol{r}=\boldsymbol{r}(t;\boldsymbol{x},t_n)$ the characteristic curve on $t\in[t_{n-1},t_n]$ defined by

$$\frac{d\boldsymbol{r}}{dt}=\frac{\boldsymbol{u}}{\phi}, \quad t_{n-1}\le t\le t_n; \quad \boldsymbol{r}|_{t=t_n}=\boldsymbol{x}. \tag{4.2}$$

Then the first two left-hand side terms of transport equation (4.1) can be rewritten in the following form [9]

$$\sqrt{\phi^2(\boldsymbol{x})+|\boldsymbol{u}(\boldsymbol{x},t_n)|^2}\,\frac{dc(\boldsymbol{x},t_n)}{d\tau}. \tag{4.3}$$

Numerically, the characteristics is backtracked from $\boldsymbol{x}$ at time step t_n to $\boldsymbol{x}^*$ at time step t_{n-1} by

$$\boldsymbol{x}^*:=\boldsymbol{x}-\frac{\boldsymbol{u}(\boldsymbol{x},t_n)}{\phi(\boldsymbol{x})}\Delta t. \tag{4.4}$$

Subsequently the first term on the left-hand side of (4.3) can be discretized by [9]

$$\sqrt{\phi^2(\boldsymbol{x})+|\boldsymbol{u}(\boldsymbol{x},t_n)|^2}\frac{dc(\boldsymbol{x},t_n)}{d\tau}\approx\phi(\boldsymbol{x})\frac{c(\boldsymbol{x},t_n)-c(\boldsymbol{x}^*,t_{n-1})}{\Delta t}. \tag{4.5}$$

Substituting (4.5) for the first term on the left-hand side of (4.3) and integrate the resulting equation against any test functions $v_h \in S_h(G)$ yields the MMOC for (4.1): find $\{c_h^n\}_{n=1}^{N_t} \subset S_h(G)$ such that

$$\begin{aligned}&\int_G \phi(\boldsymbol{x})\, \frac{c_h^n(\boldsymbol{x})-c_h^{n-1}(\boldsymbol{x}^*)}{\Delta t}\, v_h(\boldsymbol{x})d\boldsymbol{x}+\int_G \nabla v_h(\boldsymbol{x})\cdot D(\boldsymbol{x})\nabla c_h^n(\boldsymbol{x})\, d\boldsymbol{x}\\ =&\int_G f(\boldsymbol{x},t_n)v_h(\boldsymbol{x})\, d\boldsymbol{x}, \quad \forall v_h\in S_h(G), \quad 1\le n\le N_t. \end{aligned} \tag{4.6}$$

Based on the preceding discussions, we turn to the numerical discretization of the proposed model (2.1). Let $\hat{c}_h^{n-1}(\boldsymbol{x},\boldsymbol{y}) := c_h^{n-1}(\boldsymbol{x}^*,\boldsymbol{y})$ and $f^n(\boldsymbol{x},\boldsymbol{y}) := f(\boldsymbol{x},t_n,\boldsymbol{y})$. Then a similar derivation yields a stochastic MMOC for problem (2.1) by taking the inner product $\langle\cdot,\cdot\rangle$ of the scheme (4.6) for any test function $v_h \in S_h(G)\times P_N(\mathbb{R}^M)$: find $\{c_h^n\}_{n=1}^{N_t}\subset S_h(G)\times P_N(\mathbb{R}^M)$ such that for $1\le n\le N_t$

$$\begin{aligned}&\Big\langle \phi\, \frac{c_h^n-\hat{c}_h^{n-1}}{\Delta t},\, v_h\Big\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\big\langle D\nabla c_h^n,\nabla v_h\big\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ =&\big\langle f^n,v_h\big\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}, \quad \forall v_h\in S_h(G)\times P_N(\mathbb{R}^M). \end{aligned} \tag{4.7}$$

5 An optimal-order error estimate for the stochastic MMOC

We begin with a useful lemma and prove an optimal-order error estimate for the stochastic MMOC scheme to (2.1).

Lemma 5.1. [9, Lemma 1] *Let $v\in L^2(G)$ and $\hat{v}(\boldsymbol{x})=v(\boldsymbol{x}-\boldsymbol{g}(\boldsymbol{x})\Delta t)$ with $\boldsymbol{g}=(g_1,g_2)$. Assume that $g_1,g_2\in W^1_\infty(G)$. Then there exists a constant $Q>0$ such that*

$$\|v-\hat{v}\|_{H^{-1}(G)}\le Q\|v\|_{L^2(G)}\Delta t.$$

Theorem 5.1. *Assume $\phi,u_1,u_2\in W^1_\infty(G)$ with $\phi\ge\phi_0>0$, $c\in H^1\big(0,T;H^1(G;H^r_\pi(\mathbb{R}^M))\big)\cap H^1\big(0,T;L^2_{\pi_*}(\mathbb{R}^M;H^2(G))\big)\cap H^1\big(0,T;L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G))\big)$ for some integer $r\ge 0$, $\partial^2 c/\partial\tau^2\in L^2(0,T;L^2(G;L^2_\pi(\mathbb{R}^M)))$ and $c\in L^\infty(0,T;H^1(G;H^r_{\pi_*^k}(\mathbb{R}^M)))$ for $1\le k\le 2^M$ where $\{\pi_*^k\}_{k=1}^{2^M}$ correspond to all possible horizontal shifts of π_* in all directions with the distance $Q_0/2$. Then the following optimal-order estimate holds for the stochastic MMOC for Δt small enough*

$$\begin{aligned}&\|c-c_h\|_{\hat{L}^\infty(0,T;L^2(G;L^2_\pi(\mathbb{R}^M)))}+\|\nabla(c-c_h)\|_{\hat{L}^2(0,T;L^2(G;L^2_\pi(\mathbb{R}^M)))}\\ \le& QN^{-\frac{r}{2}}\Bigg[\bigg(\sum_{k=1}^{2^M}\|c\|^2_{L^\infty(0,T;H^1(G;H^r_{\pi_*^k}(\mathbb{R}^M)))}\bigg)^{1/2}+\|c\|_{H^1(0,T;H^1(G;H^r_\pi(\mathbb{R}^M)))}\Bigg]\\ &+Qh^2\big(\|c\|_{H^1(0,T;L^2_{\pi_*}(\mathbb{R}^M);H^2(G))}+\|c\|_{H^1(0,T;L^2_{\pi_{**}}(\mathbb{R}^M);H^2(G))}\big)\\ &+Q\Delta t\Big\|\frac{\partial^2 c}{\partial\tau^2}\Big\|_{L^2(0,T;L^2(G;L^2_\pi(\mathbb{R}^M)))}. \end{aligned}$$

Remark 5.1. There are regularity assumptions on the solution c in this theorem. The assumptions in space and time are roughly $c \in H^1(0,T;H^2(G)) \cap H^2(0,T;L^2(G))$, which, in the case of deterministic problems, could be guaranteed by imposing $f \in L^2(0,T;H^2(G)) \cap H^1(0,T;L^2(G))$ and $c_0 \in H^3(G)$, in addition to the smoothness assumptions on the coefficients, see e.g., [38, 41] and [10, Section 7.1.3, Theorem 6]. Furthermore, it was shown in, e.g. [19, Lemma 3.1] and [22, Theorem 3.1], that the solutions to elliptic problems with lognormal diffusivity coefficients could be sufficiently smooth in the parametric space. Therefore, we further assume some smoothness assumptions on the solutions to the proposed model in the parametric space to achieve some convergence rates. We will carry out investigations on this regularity issue for a rigorous proof in the near future.

Proof. Let $c_h^n := c_h^n(\boldsymbol{x},\boldsymbol{y})$ and $c^n := c(\boldsymbol{x},t_n,\boldsymbol{y})$. We perform the inner product $\langle\cdot,\cdot\rangle$ of the equation (2.1) and any test function $v_h \in S_h(G)\times P_N(\mathbb{R}^M)$ and subtract it from (4.7) to obtain the following error equation for $e^n = c_h^n - c^n$

$$\begin{aligned}&\langle \phi e^n, v_h\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))} + \Delta t\langle D\nabla e^n, \nabla v_h\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ =&\langle \phi \hat{e}^{n-1}, v_h\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))} + E^n(c,v_h),\end{aligned} \tag{5.1}$$

where $\hat{e}^{n-1} := e^{n-1}(\boldsymbol{x}^*,\boldsymbol{y})$ and

$$\begin{aligned}E^n(c,v_h) &= \Big\langle \Big(\sqrt{\phi^2(\boldsymbol{x}) + |\boldsymbol{u}(\boldsymbol{x},t_n)|^2}\frac{dc^n}{d\tau} - \phi(\boldsymbol{x})\frac{c^n - \hat{c}^{n-1}}{\Delta t}\Big), v_h\Big\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ &= \Big\langle \phi\int_{(x_h^*,t_{n-1})}^{(x,t_n)} \sqrt{(\boldsymbol{x}-\boldsymbol{x}^*)^2 + (\tau - t_{n-1})^2}\frac{\partial^2 c}{\partial\tau^2}d\tau, v_h\Big\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}.\end{aligned}$$

We split $e^n = \xi^n + \eta^n := (c_h^n - \mathcal{T}\mathcal{E}c^n) + (\mathcal{T}\mathcal{E}c^n - c^n)$ and choose $v_h = \xi^n$ to rewrite the error equation in terms of ξ^n and η^n as follows

$$\begin{aligned}&\langle \phi\xi^n, \xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))} + \Delta t\langle D\nabla\xi^n, \nabla\xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ =&\langle \phi\hat{\xi}^{n-1}, \xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))} - \Delta t\langle D\nabla\eta^n, \nabla\xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ &+\langle \phi(\hat{\eta}^{n-1} - \eta^n), \xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))} + E^n(c,\xi^n).\end{aligned} \tag{5.2}$$

where $\hat{\xi}^{n-1} := \xi^{n-1}(\boldsymbol{x}^*,\boldsymbol{y})$ and $\hat{\eta}^{n-1} := \eta^{n-1}(\boldsymbol{x}^*,\boldsymbol{y})$. We bound η^n by splitting it as $\eta^n = (\mathcal{T}\mathcal{E}c^n - \mathcal{T}c^n) + (\mathcal{T}c^n - c^n)$. Applying (3.15) and (3.6) we have

$$\begin{aligned}\|\eta^n\|_{L^2(G;L^2_\pi(\mathbb{R}^M))} &\le \|\mathcal{T}(\mathcal{E}c^n - c^n)\|_{L^2(G;L^2_\pi(\mathbb{R}^M))} + \|\mathcal{T}c^n - c^n\|_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ &\le Qh^2\|c^n\|_{L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G))} + QN^{-\frac{r}{2}}\|c^n\|_{L^2(G;H^r_\pi(\mathbb{R}^M))},\end{aligned} \tag{5.3}$$

and by (3.6) and (3.14)

$$\begin{aligned}\|\nabla\eta^n\|_{L^2(G;L^2_\pi(\mathbb{R}^M))} &\le \|\nabla(\mathcal{T}\mathcal{E}c^n - \mathcal{T}c^n)\|_{L^2(G;L^2_\pi(\mathbb{R}^M))} + \|\nabla(\mathcal{T}c^n - c^n)\|_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ &\le Qh\|c^n\|_{L^2_{\pi_*}(\mathbb{R}^M;H^2(G))} + QN^{-\frac{r}{2}}\|\nabla c^n\|_{L^2(G;H^r_\pi(\mathbb{R}^M))}.\end{aligned} \tag{5.4}$$

By $|d\boldsymbol{x}^*/d\boldsymbol{x}|=1+\mathcal{O}(\Delta t)$, which implies

$$\left|\frac{d\boldsymbol{x}^*}{d\boldsymbol{x}}\right|^{-1}=\frac{1}{1+\mathcal{O}(\Delta t)}\le\frac{1}{1-Q_1\Delta t}=1+\frac{Q_1\Delta t}{1-Q_1\Delta t}\le 1+2Q_1\Delta t,\quad \text{for }\ \Delta t Q_1\le\frac{1}{2},$$

the first term on the right-hand side of (5.2) can be bounded similar to [40, Equation 4.4]

$$\begin{aligned}\big|\langle\phi\hat{\xi}^{n-1},\xi^n\rangle\big| &\le\frac{1}{2}\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\frac{1}{2}\int_G\int_{\mathbb{R}^M}\pi(\boldsymbol{y})(\xi^{n-1}(\boldsymbol{x}^*,\boldsymbol{y}))^2d\boldsymbol{x}d\boldsymbol{y}\\ &=\frac{1}{2}\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\frac{1}{2}\int_G\int_{\mathbb{R}^M}\pi(\boldsymbol{y})(\xi^{n-1}(\boldsymbol{x}^*,\boldsymbol{y}))^2\left|\frac{d\boldsymbol{x}^*}{d\boldsymbol{x}}\right|^{-1}d\boldsymbol{x}^*d\boldsymbol{y}\\ &\le\frac{1}{2}\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\frac{1+Q\Delta t}{2}\|\xi^{n-1}\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}.\end{aligned}$$

For the second term on the right-hand side of (5.2), we decompose η^n by $(\mathcal{T}\mathcal{E}c^n-\mathcal{E}c^n)+(\mathcal{E}c^n-c^n)$ and apply Lemma 5.2 and (3.8) to bound

$$\begin{aligned}&\Delta t\big|\langle D\nabla\eta^n,\nabla\xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\big|\\ =&\Delta t\big|\langle D\nabla\big[(I-\mathcal{T})\mathcal{E}c^n\big],\nabla\xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\big|\\ \le& Q\Delta t N^{-r}\sum_{k=1}^{2^M}\|c^n\|^2_{H^1(G;H^r_{\pi^k_*}(\mathbb{R}^M))}+\frac{\Delta t}{2}\|(D)^{1/2}\nabla\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}.\end{aligned}\tag{5.5}$$

We bound the third term on the right-hand side of (5.2) by splitting $\eta^n-\hat{\eta}^{n-1}$ into $(\eta^n-\eta^{n-1})+(\eta^{n-1}-\hat{\eta}^{n-1})$. Then we apply (5.3) to obtain

$$\begin{aligned}\big|\langle\phi(\eta^n-\eta^{n-1}),\xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\big| &\le Q\int_{\mathbb{R}^M}\int_{t_{n-1}}^{t_n}\pi(\boldsymbol{y})\|\eta_t\|_{L^2(G)}\|\xi^n\|_{L^2(G)}dtd\boldsymbol{y}\\ &\le Q\|\eta_t\|^2_{L^2(t_{n-1},t_n;L^2(G;L^2(\mathbb{R}^M)))}+Q\Delta t\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ &\le Q\Delta t\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+Qh^4\|c_t\|^2_{L^2(t_{n-1},t_n;L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G)))}\\ &\quad+QN^{-r}\|c_t\|^2_{L^2(t_{n-1},t_n;L^2(G;H^r_\pi(\mathbb{R}^M)))}.\end{aligned}$$

To bound the second part, we apply (5.3) and Lemma 5.1 to obtain

$$\begin{aligned}&\big|\langle\phi(\eta^{n-1}-\hat{\eta}^{n-1}),\xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\big|\\ \le&\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\|\eta^{n-1}-\hat{\eta}^{n-1}\|_{H^{-1}(G)}\|\xi^n\|_{H^1(G)}d\boldsymbol{y}\\ \le& Q\Delta t\left(\frac{1}{\varepsilon}\|\eta\|^2_{L^\infty(0,T;L^2(G;L^2(\mathbb{R}^M)))}+\varepsilon\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\varepsilon\|(D)^{1/2}\nabla\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}\right)\\ \le& Q\Delta t\varepsilon\big(\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\|\nabla\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}\big)\\ &+\frac{Q\Delta t}{\varepsilon}\big(N^{-r}\|c\|_{L^\infty(0,T;L^2(G;H^r_\pi(\mathbb{R}^M)))}+h^4\|c\|_{L^\infty(0,T;L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G)))}\big).\end{aligned}\tag{5.6}$$

The last term on the right-hand side of (5.2) can be bounded by the same way in [9,40]

$$\begin{aligned}\big|E^n(c,\xi^n)\big| &\le Q(\Delta t)^{3/2}\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\|\xi^n\|_{L^2(G)}\Big\|\frac{\partial^2 c}{\partial\tau^2}\Big\|_{L^2(t_{n-1},t_n;L^2(G))}d\boldsymbol{y}\\ &\le Q\Delta t\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+Q(\Delta t)^2\Big\|\frac{\partial^2 c}{\partial\tau^2}\Big\|^2_{L^2(t_{n-1},t_n;L^2(G;L^2_\pi(\mathbb{R}^M))}.\end{aligned}$$

Let $\varepsilon=\rho_*^2/(4Q)$ and we combine all the estimates above to obtain

$$\begin{aligned}&\frac{1}{2}\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\frac{\Delta t\rho_*^2}{4}\|\nabla\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ \le&\frac{1}{2}\|\xi^{n-1}\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+Q\Delta t\big(\|\xi^{n-1}\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}\big)\\ &+Q\Delta tN^{-r}\sum_{k=1}^{2^M}\|c^n\|^2_{H^1(G;H^r_{\pi_*^k}(\mathbb{R}^M))}+Q(\Delta t)^2\Big\|\frac{\partial^2 c}{\partial\tau^2}\Big\|^2_{L^2(t_{n-1},t_n;L^2(G;L^2_\pi(\mathbb{R}^M)))}\\ &+QN^{-r}\|c\|^2_{H^1(t_{n-1},t_n;L^2(G;H^r_\pi(\mathbb{R}^M)))}+Qh^4\|c\|^2_{H^1(t_{n-1},t_n;L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G)))}\\ &+Q\Delta t\big(N^{-r}\|c\|^2_{L^\infty(0,T;L^2(G;H^r_\pi(\mathbb{R}^M)))}+h^4\|c\|^2_{L^\infty(0,T;L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G)))}\big).\end{aligned}\tag{5.7}$$

Then we sum (5.7) for $n=1,\cdots,N_1(\le N_t)$ and cancel like terms to obtain

$$\begin{aligned}&\|\xi^{N_1}\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+\frac{\Delta t\rho_*^2}{4}\sum_{n=1}^{N_1}\|\nabla\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\ \le&Q\Delta t\sum_{n=0}^{N_1}\|\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}+QN^{-r}\sum_{k=1}^{2^M}\|c\|^2_{L^\infty(0,T;H^1(G;H^r_{\pi_*^k}(\mathbb{R}^M)))}\\ &+QN^{-r}\|c\|^2_{H^1(0,T;L^2(G;H^r_\pi(\mathbb{R}^M)))}+Qh^4\|c\|^2_{H^1(0,T;L^2_{\pi_{**}}(\mathbb{R}^M;H^2(G)))}\\ &+Q(\Delta t)^2\Big\|\frac{\partial^2 c}{\partial\tau^2}\Big\|^2_{L^2(0,T;L^2(G;L^2_\pi(\mathbb{R}^M)))}.\end{aligned}\tag{5.8}$$

Finally we apply the Gronwall's inequality and incorporate (5.1) and the estimates (5.3)-(5.4) of η^n to complete the proof. ☐

Lemma 5.2. *Under the conditions of Theorem* 5.1, *the estimate* (5.5) *holds.*

Proof. We apply the Cauchy's inequality and the estimate

$$\rho(\boldsymbol{y})=\rho_{**}+\rho_{**}e^{C(\bar{Y})}\exp\Big(\sum_{i=1}^M|y_i|Q_0\Big)\le 2\rho_{**}e^{C(\bar{Y})}\exp\Big(\sum_{i=1}^M|y_i|Q_0\Big)\le Q\exp\Big(\sum_{i=1}^M|y_i|Q_0\Big)$$

to get

$$
\begin{aligned}
&\Delta t\big|\langle D\nabla\big[(I-\mathcal{T})\mathcal{E}c^n\big],\nabla\xi^n\rangle_{L^2(G;L^2_\pi(\mathbb{R}^M))}\big|\\
\le&\Delta t\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\|D^{1/2}(I-\mathcal{T})\nabla\mathcal{E}c^n\|_{L^2(G)}\|D^{1/2}\nabla\xi^n\|_{L^2(G)}d\boldsymbol{y}\\
\le&\frac{\Delta t}{2}\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\rho(\boldsymbol{y})\int_G\big((I-\mathcal{T})\nabla\mathcal{E}c^n\big)^2d\boldsymbol{x}d\boldsymbol{y}+\frac{\Delta t}{2}\|D^{1/2}\nabla\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}\\
\le&Q\Delta t\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\int_G\exp\Big(\sum_{i=1}^M|y_i|Q_0\Big)\big((I-\mathcal{T})\nabla\mathcal{E}c^n\big)^2d\boldsymbol{x}d\boldsymbol{y}\\
&+\frac{\Delta t}{2}\|(D)^{1/2}\nabla\xi^n\|^2_{L^2(G;L^2_\pi(\mathbb{R}^M))}.
\end{aligned}\tag{5.9}
$$

In each direction y_i of $\boldsymbol{y}$, we split the corresponding integral domain $\mathbb{R}$ into the union of $R_i^-:=(-\infty,0)$ and $R_i^+:=[0,\infty)$ in order to remove the absolute value of y_i on the exponential in (5.9). In this way the integral on $\mathbb{R}^M$ are split into a sum of 2^M sub-integrals labeled by $k=1,\cdots,2^M$ and each of them integrates on the union of either R_i^+ or R_i^- for $1\le i\le M$. Conventionally, we apply the graded lexicographic ordering of the multi-index of dimension M on domains of the sub-integrals with $R_1^-\times\cdots\times R_M^-$ as the first element. Then, for the first sub-integral, we replace each $|y_i|$ by $-y_i$ and apply (3.6) and the variable substitution $\boldsymbol{z}=\boldsymbol{y}+Q_0\boldsymbol{I}/2$ for $\boldsymbol{I}:=(1,\cdots,1)$ as well as the following estimate for $\tilde{c}^n(\boldsymbol{x},\boldsymbol{z}):=c(\boldsymbol{x},t_n,\boldsymbol{z}+Q_0\boldsymbol{I}/2)$

$$
\begin{aligned}
\|\nabla\mathcal{E}\tilde{c}^n\|^2_{L^2(G;H^r_\pi(\mathbb{R}^M))}&=\sum_{|\boldsymbol{l}|=0}^r\int_G\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\Big(\frac{d^{|\boldsymbol{l}|}}{d\boldsymbol{y}^{\boldsymbol{l}}}(\nabla\mathcal{E}\tilde{c}^n)\Big)^2d\boldsymbol{y}d\boldsymbol{x}\\
&=\sum_{|\boldsymbol{l}|=0}^r\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\Big\|\nabla\mathcal{E}\Big(\frac{d^{|\boldsymbol{l}|}}{d\boldsymbol{y}^{\boldsymbol{l}}}\tilde{c}^n\Big)\Big\|^2_{L^2(G)}d\boldsymbol{y}\\
&\le Q\sum_{|\boldsymbol{l}|=0}^r\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\rho(\boldsymbol{y})\Big\|\nabla\frac{d^{|\boldsymbol{l}|}}{d\boldsymbol{y}^{\boldsymbol{l}}}\tilde{c}^n\Big\|^2_{L^2(G)}d\boldsymbol{y}\quad\text{(using (3.12))}\\
&=Q\int_G\sum_{|\boldsymbol{l}|=0}^r\int_{\mathbb{R}^M}\pi_*(\boldsymbol{z}-Q_0\boldsymbol{I}/2)\Big(\nabla\frac{d^{|\boldsymbol{l}|}}{d\boldsymbol{z}^{\boldsymbol{l}}}c^n\Big)^2d\boldsymbol{z}d\boldsymbol{x}\\
&=Q\|\nabla c^n\|^2_{L^2(G;H^r_{\pi_*^1}(\mathbb{R}^M))},\quad\pi_*^1(\boldsymbol{z}):=\pi_*(\boldsymbol{z}-Q_0\boldsymbol{I}/2),
\end{aligned}
$$

where π_* is defined by (3.13) that includes the ρ, to obtain

$$
\begin{aligned}
&\Delta t\int_{R_1^-\times\cdots\times R_M^-}\pi(\boldsymbol{y})\int_G\exp\Big(-\sum_{i=1}^M y_iQ_0\Big)\big((I-\mathcal{T})\nabla\mathcal{E}c^n\big)^2d\boldsymbol{x}d\boldsymbol{y}\\
\le&\Delta t\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\int_G\exp\Big(-\sum_{i=1}^M y_iQ_0\Big)\big((I-\mathcal{T})\nabla\mathcal{E}c^n\big)^2d\boldsymbol{x}d\boldsymbol{y}
\end{aligned}
$$

$$
\begin{aligned}
&= \Delta t \exp\Big(\sum_{i=1}^{M}(Q_0/2)^2\Big)\int_{\mathbb{R}^M}\pi(\boldsymbol{z})\int_G \big((I-\mathcal{T})\nabla\mathcal{E}\tilde{c}^n\big)^2 d\boldsymbol{x}d\boldsymbol{z} \\
&\le Q\Delta t N^{-r}\|\nabla\mathcal{E}\tilde{c}^n\|^2_{L^2(G;H^r_\pi(\mathbb{R}^M))} \le Q\Delta t N^{-r}\|\nabla c^n\|^2_{L^2(G;H^r_{\pi^1_*}(\mathbb{R}^M))}.
\end{aligned}
$$

Similarly, we define π^k_* for $1\le k\le 2^M$ according to the aforementioned ordering and consequently, we bound the first term on the right-hand side of (5.9) by

$$
Q\Delta t\int_{\mathbb{R}^M}\pi(\boldsymbol{y})\int_G \exp\Big(\sum_{i=1}^{M}|y_i|Q_0\Big)\big((I-\mathcal{T})\nabla\mathcal{E}c^n\big)^2 d\boldsymbol{x}d\boldsymbol{y} \le Q\Delta t N^{-r}\sum_{k=1}^{2^M}\|\nabla c^n\|^2_{L^2(G;H^r_{\pi^k_*}(\mathbb{R}^M))},
$$

which completes the proof. □

6 Numerical experiments

We carry out numerical experiments to investigate the performance of the stochastic MMOC scheme. Let $G=[-0.5,0.5]^2$, $\boldsymbol{u}(x_1,x_2)=(-4x_2,4x_1)$ and $[0,T]=[0,\pi/2]$, a time period of a complete rotation. We set $\phi=0.3$, $\rho_0=\rho_1=0.3\times10^{-4}$, $\bar{Y}=1\times10^{-2}$, $M=3$ and $f\equiv0$. The initial condition is given by

$$
u_0=\exp\Big(-\frac{(x_1-x_{1,c})^2+(x_2-x_{2,c})^2}{2\sigma^2}\Big),
$$

where $(x_{1,c},x_{2,c})=(-0.1,0)$ and $\sigma=0.0447$ are the center and standard derivation of the Gaussian pulse, respectively. In the experiments, the sparse polynomial space (3.7) will be applied combined with the rectangular element with uniform partitions for both space and time. The numerical solution c_{MC} of the Monte Carlo method using 5000 samplings and $h=1/128$ and $\Delta t=\pi/64$ serves as the reference solution and the errors are measured in $\|\mathbb{E}(c_h)-\mathbb{E}(c_{MC})\|_{\hat{L}^\infty(0,T;L^2(G))}$ where $\mathbb{E}(\cdot)$ denotes the probabilistic expectation [35]. It is clear that the error can be bounded by $Q\|c_h-c_{MC}\|_{\hat{L}^\infty(0,T;L^2(G);L^2_\pi(\mathbb{R}^M))}$, which was estimated in Theorem 5.1. We accordingly measure the convergence rates α, β, and γ of the stochastic MMOC scheme with respect to the spatial mesh size h, time step size Δt, and the spectral polynomial degree N

$$
\|\mathbb{E}(c_h)-\mathbb{E}(c_{MC})\|_{\hat{L}^\infty(0,T;L^2(G))}\le Q\big(h^\alpha+(\Delta t)^\beta+N^{-\gamma}\big).
$$

We expect a second order convergence in space and first order in time. The order γ depends on the regularity of the solutions on the stochastic space, the exact value of which is hard to determine. For this reason, we instead measure the quotients of the errors under different N as the decay rate.

We present the reference solution $\mathbb{E}(c_{MC})(\boldsymbol{x},T)$ and the numerical solution $\mathbb{E}(c_h^{N_t})(\boldsymbol{x})$ solved under $h=1/60$, $\Delta t=\pi/64$ and $N=2$ in Fig. 1 and Fig. 2, respectively, which show

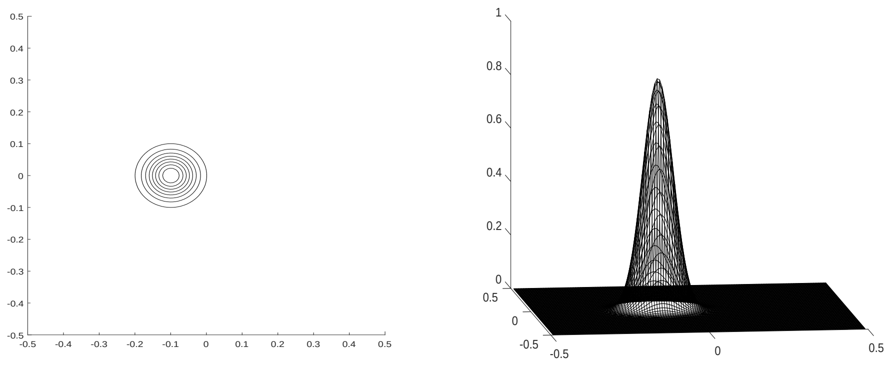

Figure 1: $\mathbb{E}(c_{MC})(\boldsymbol{x},T)$ solved under $h=1/128$ and $\Delta t=\pi/64$ from the view of top (left) and side (right).

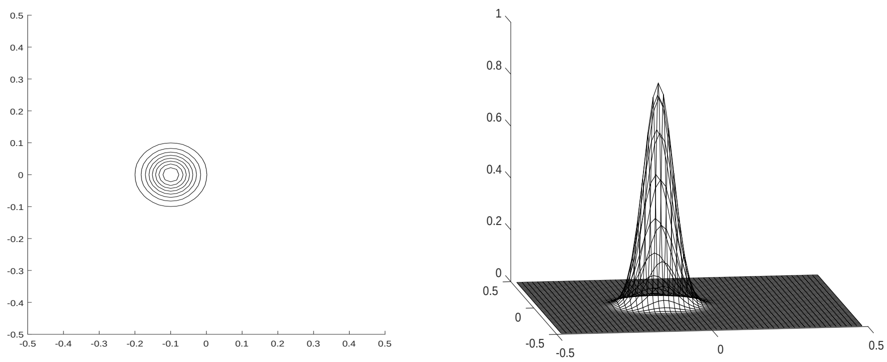

Figure 2: $\mathbb{E}(c_h^{N_t})(\boldsymbol{x})$ solved under $h=1/60$, $\Delta t=\pi/64$ and $N=2$ from the view of top (left) and side (right).

that the stochastic MMOC accurately captures the revolving interface of the Gaussian pulse with small polynomial degrees and thus demonstrate the effectiveness of the proposed method for the advection-dominated problems. In Table 1, the sharp decay rate indicates the fast convergence of the stochastic MMOC in the stochastic space and the results in Table 2 are consistent with the error estimates in Theorem 5.1. Furthermore, we observe from Table 2 that large time steps can be used without loss of accuracy, which

Table 1: Convergence of stochastic MMOC under $\Delta t=\pi/64$.

N	$h=1/40$	Decay rate	$h=1/60$	Decay rate
0	8.43E-02		8.58E-02	
1	8.16E-03	1/10.33	8.30E-03	1/10.34
2	1.01E-03	1/8.08	1.03E-03	1/8.06

Table 2: Convergence of stochastic MMOC under $N=2$.

h	$\Delta t=\pi/64$	Δt	$h=1/40$
1/10	6.48E-02	$\pi/10$	3.02E-03
1/20	2.41E-02	$\pi/12$	2.41E-03
1/30	8.08E-03	$\pi/14$	1.87E-03
1/40	2.83E-03	$\pi/16$	1.51E-03
1/50	1.75E-03	$\pi/18$	1.30E-03
1/60	1.60E-03	$\pi/20$	1.27E-03
Conv. rate	α=2.25		β=1.32

exhibits the advantage of the method of characteristics and demonstrates its strong potential for the long-time simulation.

7 Concluding remarks

In this paper we develop and analyze a stochastic MMOC method for a time-dependent advection-diffusion equation modeling solute transport in randomly heterogeneous porous media. Error estimates were rigorously proved and numerical experiments were performed. Further generalizations of the proposed model may be the coupled miscible displacement system [11, 15, 24] with non-smooth randomness or noises, which significantly increases the difficulties of analysis and simulations due to, e.g., the coupling effect of the equations and the low regularity of the solutions. Another possible improvement may lie in the refinement of the estimate in Lemma 5.2 in order that the 2^M multiple of the errors in (5.5) could be reduced or removed. Currently, we did not find a straightforward way to remove this exponential dependence, and some significant modifications may be needed to achieve this goal. We will carry out investigations for these extensions and improvements in the near future.

A potential alternative approach to derive error estimates in Theorem 5.1 is to firstly derive the path-wise convergence rate for the MMOC scheme, which may be obtained from the existing numerical analysis results for deterministic problems, and then take the expectation for the resulting estimates. The idea leads to an alternative discretization but may introduce additional numerical analysis difficulties in recovering the results in Theorem 5.1. Due to the coupling of the stochastic variables and the spatially-dependent functions in the diffusivity coefficient and its nonlinearity, the proposed Galerkin approach (4.7) generates a global approximation in a coupling and all-at-once manner with interactions among different basis. How to accommodate these coupling effects and interactions from path-wise estimates is an interesting but challenging problem and we plan to investigate this approach in the near future.

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