



INDUSTRIAL
MATHEMATICS
INSTITUTE

2001:20

An optimal-order error estimate
for MMOC and MMOCOA
schemes for multidimensional
advection-reaction equations

H. Wang

IMI

Preprint Series

Department of Mathematics
University of South Carolina

An Optimal-Order Error Estimate for MMOC and MMOCAA Schemes for Multidimensional Advection-Reaction Equations

Hong Wang

*Department of Mathematics
University of South Carolina
Columbia, South Carolina 29208*

In this paper, we analyze the modified method of characteristics (MMOC) and an improved version of the MMOC, named the modified method of characteristics with adjusted advection (MMOCAA), for multidimensional advection-reaction transport equations in a uniform manner. We derive an optimal-order error estimate for these schemes. Numerical results are presented to verify the theoretical estimates.

Keywords: advection-reaction equations; characteristic methods; Eulerian-Lagrangian methods; error estimates; the modified method of characteristics; the modified method of characteristics with adjusted advection

I. INTRODUCTION

Advection-dominated transport partial differential equations (PDEs) arise in petroleum reservoir simulation, subsurface contaminant transport and many other important applications [1, 9]. The numerical treatment of these equations often presents severe difficulties. Standard finite difference or finite element methods or upwind schemes tend to generate numerical solutions with severe nonphysical oscillation or excessive numerical diffusion. The modified method of characteristics (MMOC) was first formulated for an advection-diffusion equation by Douglas and Russell in [7] and then extended by Russell [13] to nonlinear coupled systems in two and three spatial dimensions. Similar schemes have been developed by Pironneau [12] for the incompressible Navier-Stokes equations, and by Benque and Ronat [2] and by Morton, Priestley, and Süli [11] for advection-dominated transport equations.

In the MMOC scheme, the time derivative and the advection term are combined as a directional derivative along the characteristics, leading to a characteristic time-stepping procedure. Consequently, the MMOC symmetrizes and stabilizes the governing PDEs, and allows for large time steps in a simulation without the loss of accuracy and

eliminates the excessive numerical dispersion and grid orientation effects present in many upwind methods. An algorithm combining the mixed finite element method and the MMOC scheme has been successfully applied to the miscible displacement problem in porous media by Ewing, Russell, and Wheeler [10]. Recently, in the simulation of two-phase immiscible flow in porous media, Douglas, Furtado, and Pereira [5] formulated an improved version of the MMOC, named the modified method of characteristics with adjusted advection (MMOCAA), to correct the mass balance error of the MMOC by a higher-order perturbation of the foot of the characteristics. Douglas, Huang, Pereira [6] derived appropriate forms of the MMOCAA schemes for advection-diffusion problems. The MMOCAA scheme conserves mass and preserves the conceptual and computational advantages of the MMOC scheme.

For advection-dominated equations with nondegenerate diffusion, optimal-order convergence rates of $\mathcal{O}(h^{k+1} + \Delta t)$ in L^2 at each time level for the MMOC scheme was proved in [7] by Douglas and Russell, where k is the degree of the piecewise polynomial approximating space. But these estimates fall short for the MMOC scheme for pure advection problems. The error estimate for the MMOC applied to periodic linear advection problems in multiple space dimensions is at best $\mathcal{O}(h^k + \Delta t)$ in L^2 [4], which is a suboptimal-order error estimate in the sense that the power of h is one lower than is possible for a best approximation. Recently, Douglas, Huang, and Pereira [6] obtained a suboptimal-order L^2 error estimate of $\mathcal{O}(h + \Delta t)$ for the piecewise-linear MMOCAA scheme for an advection-diffusion equation with nondegenerate diffusion.

In this paper we analyze the piecewise-linear MMOC and MMOCAA schemes for multidimensional advection-reaction equations uniformly and prove an optimal-order L^2 error estimate for these schemes. The rest of this paper is organized as follows: In section II, we briefly review the MMOC and MMOCAA formulation. In section III, we prove the main error estimate. In section IV, we prove an auxiliary lemma which is crucial in deriving the optimal-order error estimate. In section V, we perform numerical experiments to verify the theoretical estimates.

II. THE MMOC AND MMOCAA FORMULATIONS

We consider the following two-dimensional linear advection-reaction equation

$$\begin{aligned} \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c + Rc &= f(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Omega \times (0, T], \\ c(\mathbf{x}, 0) &= c_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \end{aligned} \quad (2.1)$$

where $\Omega = (a, b) \times (c, d)$ is a rectangular domain. $\mathbf{u}(\mathbf{x}, t) = (V_1(\mathbf{x}, t), V_2(\mathbf{x}, t))$ is a velocity field, $R(\mathbf{x}, t)$ is a first-order reaction coefficient, $f(\mathbf{x}, t)$ is a given function describing source terms, and $c(\mathbf{x}, t)$ is the unknown function representing the solute concentration of a dissolved substance. For convenience, we assume that problem (2.1) is Ω -periodic, i.e., we assume that all functions in (2.1) are spatially Ω -periodic [5, 6].

A. Preliminaries and notation

On the spatial domain Ω , we define the following Sobolev spaces

$$L^2(\Omega) = \left\{ f(\mathbf{x}) \mid \int_{\Omega} f^2(\mathbf{x}) d\mathbf{x} < \infty \right\},$$

$$L^\infty(\Omega) = \left\{ f(\mathbf{x}) \mid \operatorname{ess\,sup}_{\mathbf{x} \in \Omega} |f(\mathbf{x})| < \infty \right\},$$

$$H^m(\Omega) = \left\{ f(\mathbf{x}) \mid \frac{\partial^{|\boldsymbol{\alpha}|} f(\mathbf{x})}{\partial \mathbf{x}^{\boldsymbol{\alpha}}} \in L^2(\Omega), |\boldsymbol{\alpha}| \leq m \right\},$$

where the multi-index $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)$, $|\boldsymbol{\alpha}| = \alpha_1 + \alpha_2$, and the norms are given by

$$\|f\|_{L^2(\Omega)} = \left[\int_{\Omega} f^2(\mathbf{x}) d\mathbf{x} \right]^{1/2}, \quad \|f\|_{L^\infty(\Omega)} = \operatorname{ess\,sup}_{\mathbf{x} \in \Omega} |f(\mathbf{x})|,$$

$$\|f\|_{H^m(\Omega)} = \sum_{|\boldsymbol{\alpha}| \leq m} \left\| \frac{\partial^{|\boldsymbol{\alpha}|} f(\mathbf{x})}{\partial \mathbf{x}^{\boldsymbol{\alpha}}} \right\|_{L^2(\Omega)}.$$

We will drop the domain Ω in these notations when it is clear. In addition, we also use the following spaces that incorporate time dependence for any spaces \mathcal{X} defined on Ω

$$L^p(t_1, t_2; \mathcal{X}) = \left\{ w(\mathbf{x}, t) \mid \|w(\cdot, t)\|_{\mathcal{X}} \in L^p(t_1, t_2) \right\}$$

$$H^m(t_1, t_2; \mathcal{X}) = \left\{ w(\mathbf{x}, t) \mid \sum_{0 \leq |\boldsymbol{\alpha}| \leq m} \int_{t_1}^{t_2} \left\| \frac{\partial^{\boldsymbol{\alpha}} w}{\partial t}(\cdot, t) \right\|_{\mathcal{X}}^2 dt < \infty \right\},$$

with the norms

$$\|w\|_{L^p(t_1, t_2; \mathcal{X})} = \left\| \|w(\cdot, t)\|_{\mathcal{X}} \right\|_{L^p(t_1, t_2)}, \quad 1 \leq p \leq +\infty,$$

$$\|w\|_{H^m(t_1, t_2; \mathcal{X})} = \left[\sum_{0 \leq |\boldsymbol{\alpha}| \leq m} \int_{t_1}^{t_2} \left\| \frac{\partial^{\boldsymbol{\alpha}} w}{\partial t}(\cdot, t) \right\|_{\mathcal{X}}^2 dt \right]^{1/2}.$$

We define a partition of the time interval $[0, T]$ by

$$t_m = m\Delta t, \quad m = 0, 1, \dots, M, \quad \text{with} \quad \Delta t = \frac{T}{M}, \quad (2.2)$$

and a discrete time-dependent norm

$$\|w\|_{\hat{L}^\infty(0, T; \mathcal{X})} = \max_{0 \leq m \leq M} \|w(\cdot, t_m)\|_{\mathcal{X}}.$$

B. The Modified Method of Characteristics (MMOC)

In the modified method of characteristics, the time derivative and the advection term in Eq. (2.1) is written as a directional derivative

$$\frac{\partial c}{\partial t}(\mathbf{x}, t_m) + \mathbf{u}(\mathbf{x}, t_m) \cdot \nabla c(\mathbf{x}, t_m) = \sqrt{1 + |\mathbf{u}(\mathbf{x}, t_m)|^2} \frac{\partial c}{\partial \tau}(\mathbf{x}, t_m),$$

along the characteristic $\mathbf{r}(\tau; \mathbf{x}, t_m)$ defined by

$$\frac{d\mathbf{r}}{d\tau} = \mathbf{u}(\mathbf{r}, \tau), \quad \mathbf{r}(\tau; \mathbf{x}, t_m) \Big|_{\tau=t_m} = \mathbf{x}.$$

Then the directional derivative $\frac{\partial c}{\partial \tau}(\mathbf{x}, t_m)$ along the characteristic $\mathbf{r}(\tau; \mathbf{x}, t_m)$ is approximated by a backward difference quotient along the approximate characteristic in the

time stepping procedure [7]

$$\sqrt{1 + |\mathbf{u}(\mathbf{x}, t_m)|^2} \frac{\partial c}{\partial \tau}(\mathbf{x}, t_m) = \frac{c(\mathbf{x}, t_m) - c(\mathbf{x}^*, t_{m-1})}{\Delta t} + E_1(c(\mathbf{x}, t_m)), \quad (2.3)$$

where

$$\mathbf{x}^* = \mathbf{x} - \mathbf{u}(\mathbf{x}, t_m)\Delta t,$$

$$E_1(c(\mathbf{x}, t_m)) = \sqrt{1 + |\mathbf{u}(\mathbf{x}, t_m)|^2} \frac{\partial c}{\partial \tau}(\mathbf{x}, t_m) - \frac{c(\mathbf{x}, t_m) - c(\mathbf{x}^*, t_{m-1})}{\Delta t}. \quad (2.4)$$

A weak formulation for problem (2.1) states as follows: Find $c(\mathbf{x}, t_m) \in H^1(\Omega)$ for $m = 1, 2, \dots, M$, such that for any $w(\mathbf{x}) \in H^1(\Omega)$

$$\begin{aligned} & \int_{\Omega} \frac{c(\mathbf{x}, t_m) - c(\mathbf{x}^*, t_{m-1})}{\Delta t} w(\mathbf{x}) d\mathbf{x} + \int_{\Omega} R(\mathbf{x}, t_m) c(\mathbf{x}, t_m) w(\mathbf{x}) d\mathbf{x} \\ & = \int_{\Omega} f(\mathbf{x}, t_m) w(\mathbf{x}) d\mathbf{x} + \int_{\Omega} E_1(c(\mathbf{x}, t_m)) w(\mathbf{x}) d\mathbf{x}. \end{aligned} \quad (2.5)$$

We introduce a uniform rectangular partition on Ω by

$$\begin{aligned} \mathcal{T}^x : x_i &= a + i\Delta x, \quad i = 1, 2, \dots, I, \quad \text{with} \quad \Delta x = \frac{b-a}{I}, \\ \mathcal{T}^y : y_j &= a + j\Delta y, \quad j = 1, 2, \dots, J, \quad \text{with} \quad \Delta y = \frac{d-c}{J}. \end{aligned} \quad (2.6)$$

Let $h = [(\Delta x)^2 + (\Delta y)^2]^{1/2}$ be the diameter of the partition, we assume that the partition is quasi-uniform, i.e.,

$$1 \leq \frac{h}{\min\{\Delta x, \Delta y\}} \leq M_1 < +\infty.$$

Let $\mathcal{S}_h(\Omega)$ be the continuous and piecewise-bilinear finite element space on Ω with the partition in (2.6) and is Ω -periodic. Then the MMOC scheme states as follows: Find $c_h(\mathbf{x}, t_m) \in \mathcal{S}_h(\Omega)$ for $m = 1, 2, \dots, M$, such that

$$\begin{aligned} & \int_{\Omega} \frac{c_h(\mathbf{x}, t_m) - c_h(\mathbf{x}^*, t_{m-1})}{\Delta t} w_h(\mathbf{x}) d\mathbf{x} + \int_{\Omega} R(\mathbf{x}, t_m) c_h(\mathbf{x}, t_m) w_h(\mathbf{x}) d\mathbf{x} \\ & = \int_{\Omega} f(\mathbf{x}, t_m) w_h(\mathbf{x}) d\mathbf{x}, \quad \forall w_h(\mathbf{x}) \in \mathcal{S}_h(\Omega). \end{aligned} \quad (2.7)$$

The MMOC scheme (2.7) follows the flow by tracking the characteristics backward from a point \mathbf{x} in a fixed grid at the time step t_m to a point \mathbf{x}^* at the previous time step t_{m-1} . Hence, the MMOC avoids the grid distortion problems present in forward tracking methods. Unfortunately, MMOC fails to conserve mass.

C. The Modified Method of Characteristics with Adjusted Advection (MMOCAA)

Here we briefly outline the idea of the MMOCAA and refer readers to [5, 6] for the detailed development and description. Summing the MMOC scheme (2.7) for all the test functions, we obtain

$$\begin{aligned} & \int_{\Omega} c_h(\mathbf{x}, t_m) d\mathbf{x} + \Delta t \int_{\Omega} R(\mathbf{x}, t_m) c_h(\mathbf{x}, t_m) d\mathbf{x} \\ & = \int_{\Omega} c_h(\mathbf{x}^*, t_{m-1}) d\mathbf{x} + \Delta t \int_{\Omega} f(\mathbf{x}, t_m) d\mathbf{x}. \end{aligned} \quad (2.8)$$

On the other hand, integrating Eq. (2.1) over the space-time strip $\Omega \times [t_{m-1}, t_m]$ and applying the divergence theorem, we obtain

$$\begin{aligned} & \int_{\Omega} c(\mathbf{x}, t_m) d\mathbf{x} + \int_{t_{m-1}}^{t_m} \int_{\Omega} [-\nabla \cdot \mathbf{u}(\mathbf{x}, t) + R(\mathbf{x}, t)] c(\mathbf{x}, t) d\mathbf{x} dt \\ &= \int_{\Omega} c(\mathbf{x}, t_{m-1}) d\mathbf{x} + \int_{t_{m-1}}^{t_m} \int_{\Omega} f(\mathbf{x}, t) d\mathbf{x} dt. \end{aligned} \quad (2.9)$$

Applying Euler quadrature at time t_m to evaluate the space-time integrals in Eq. (2.9), and then taking $c(\mathbf{x}, t_{m-1}) = c_h(\mathbf{x}, t_{m-1})$, we obtain the following equation of mass conservation in the integral form (up to the order of the truncation error)

$$\begin{aligned} & \int_{\Omega} \left\{ 1 + \Delta t [-\nabla \cdot \mathbf{u}(\mathbf{x}, t_m) + R(\mathbf{x}, t_m)] \right\} c(\mathbf{x}, t_m) d\mathbf{x} \\ &= \int_{\Omega} c_h(\mathbf{x}, t_{m-1}) d\mathbf{x} + \Delta t \int_{\Omega} f(\mathbf{x}, t_m) d\mathbf{x}. \end{aligned} \quad (2.10)$$

Eq. (2.8) is the equation of the mass conservation, which the MMOC solution $c_h(\mathbf{x}, t_m)$ satisfies for the given initial condition $c_h(\mathbf{x}, t_{m-1})$ at time t_{m-1} . In contrast, Eq. (2.10) specifies the true (up to the local truncation error) mass conservation equation which the exact solution $c(\mathbf{x}, t_m)$ of (2.1), starting from the initial condition $c_h(\mathbf{x}, t_{m-1})$ at time t_{m-1} , satisfies. Let

$$\begin{aligned} Q_{m-1} &= \int_{\Omega} c_h(\mathbf{x}, t_{m-1}) d\mathbf{x} + \Delta t \int_{\Omega} \nabla \cdot \mathbf{u}(\mathbf{x}, t_m) c(\mathbf{x}, t_m) d\mathbf{x}, \\ Q_{m-1}^* &= \int_{\Omega} c_h(\mathbf{x}^*, t_{m-1}) d\mathbf{x}. \end{aligned}$$

From Eqs. (2.8) and (2.10), we see that to maintain mass balance we must have $Q_{m-1} = Q_{m-1}^*$. Because $c(\mathbf{x}, t_m)$ is unknown in the evaluation of Q_{m-1} , it is approximated by an extrapolation of $2c_h(\mathbf{x}, t_{m-1}) - c_h(\mathbf{x}, t_{m-2})$.

If $Q_{m-1} \neq Q_{m-1}^*$, we see that the MMOC scheme (2.7) will introduce mass balance error. To correct this error, the following higher-order perturbations \mathbf{x}_+^* and \mathbf{x}_-^* of \mathbf{x}^* are defined for some fixed constant $\kappa > 0$

$$\begin{aligned} \mathbf{x}_+^* &= \mathbf{x} - \mathbf{u}(\mathbf{x}, t_m) \Delta t + \kappa \mathbf{u}(\mathbf{x}, t_m) (\Delta t)^2 = \mathbf{x}^* + \kappa \mathbf{u}(\mathbf{x}, t_m) (\Delta t)^2, \\ \mathbf{x}_-^* &= \mathbf{x} - \mathbf{u}(\mathbf{x}, t_m) \Delta t - \kappa \mathbf{u}(\mathbf{x}, t_m) (\Delta t)^2 = \mathbf{x}^* - \kappa \mathbf{u}(\mathbf{x}, t_m) (\Delta t)^2. \end{aligned} \quad (2.11)$$

Then we let

$$c_h^{\#}(\mathbf{x}^*, t_{m-1}) = \begin{cases} \max\{c_h(\mathbf{x}_+^*, t_{m-1}), c_h(\mathbf{x}_-^*, t_{m-1})\}, & \text{if } Q_{m-1}^* \leq Q_{m-1}, \\ \min\{c_h(\mathbf{x}_+^*, t_{m-1}), c_h(\mathbf{x}_-^*, t_{m-1})\}, & \text{if } Q_{m-1}^* > Q_{m-1}, \end{cases} \quad (2.12)$$

and set

$$Q_{m-1}^{\#} = \int_{\Omega} c_h^{\#}(\mathbf{x}^*, t_m) d\mathbf{x}.$$

Then one needs to find θ_{m-1} such that

$$Q_{m-1} = \theta_{m-1} Q_{m-1}^* + (1 - \theta_{m-1}) Q_{m-1}^{\#},$$

and let

$$\check{c}_h(\mathbf{x}^*, t_{m-1}) = \theta_{m-1} c_h(\mathbf{x}^*, t_{m-1}) + (1 - \theta_{m-1}) c_h^\#(\mathbf{x}^*, t_{m-1}). \quad (2.13)$$

Then, one has

$$\int_{\Omega} \check{c}_h(\mathbf{x}^*, t_{m-1}) d\mathbf{x} = Q_{m-1}.$$

In the MMOC scheme one replaces the $c_h(\mathbf{x}^*, t_{m-1})$ term in the MMOC scheme (2.7) by $\check{c}_h(\mathbf{x}^*, t_{m-1})$. Consequently, the MMOC scheme conserves mass globally.

III. ERROR ESTIMATES FOR THE MMOC AND MMOC AA SCHEMES

In this section we derive optimal-order error estimates for the MMOC and MMOC AA schemes. We notice that the only difference of the MMOC AA scheme from the MMOC scheme is that in the $c_h(\mathbf{x}^*, t_{m-1})$ term in the MMOC scheme (2.7) the \mathbf{x}^* is possibly replaced by one of its higher-order perturbations \mathbf{x}_+^* and \mathbf{x}_-^* defined in (2.11). Hence, we can analyze both schemes in a uniform manner, with the understanding that in the MMOC AA scheme the \mathbf{x}^* could be one of the \mathbf{x}_+^* and \mathbf{x}_-^* .

Let $\Pi : C(\bar{\Omega}) \rightarrow \mathcal{S}_h(\Omega)$ be the piecewise-bilinear interpolation operator. For $m = 0, 1, \dots, M$, we define

$$\begin{aligned} e(\mathbf{x}, t_m) &= c_h(\mathbf{x}, t_m) - c(\mathbf{x}, t_m), & \xi(\mathbf{x}, t_m) &= c_h(\mathbf{x}, t_m) - \Pi c(\mathbf{x}, t_m), \\ \eta(\mathbf{x}, t_m) &= \Pi c(\mathbf{x}, t_m) - c(\mathbf{x}, t_m) \end{aligned} \quad (3.1)$$

to be the global truncation error, the error between the numerical solution c_h and the piecewise-bilinear interpolation Πc , and the piecewise-bilinear interpolation error $\Pi c - c$, respectively. It is well known that the following estimates hold [3]

$$\begin{aligned} \|\Pi f - f\|_{L^2(\Omega)} &\leq M h^2 \|f\|_{H^2(\Omega)}, & \forall f \in H^2(\Omega), \\ \|f_h\|_{L^\infty(\Omega)} &\leq M h^{-1} \|f_h\|_{L^2(\Omega)}, & \forall f_h \in \mathcal{S}_h(\Omega). \end{aligned} \quad (3.2)$$

Subtracting the MMOC scheme (2.7) from the reference equation (2.5) and choosing the test function $w(x) = \xi(\mathbf{x}, t_m)$, we obtain the following error equation

$$\begin{aligned} \int_{\Omega} \frac{e(\mathbf{x}, t_m) - e(\mathbf{x}^*, t_{m-1})}{\Delta t} \xi(\mathbf{x}, t_m) d\mathbf{x} + \int_{\Omega} R(\mathbf{x}, t_m) e(\mathbf{x}, t_m) \xi(\mathbf{x}, t_m) d\mathbf{x} \\ = - \int_{\Omega} E_1(c(\mathbf{x}, t_m)) \xi(\mathbf{x}, t_m) d\mathbf{x}. \end{aligned} \quad (3.3)$$

Since the interpolation error $\eta(\mathbf{x}, t_m)$ is given by (3.2), we only need to estimate $\xi(\mathbf{x}, t_m)$ by rewriting Eq. (3.3) in terms of ξ and η as follows

$$\begin{aligned} \int_{\Omega} \xi^2(\mathbf{x}, t_m) d\mathbf{x} &= \int_{\Omega} \xi(\mathbf{x}^*, t_{m-1}) \xi(\mathbf{x}, t_m) d\mathbf{x} + \int_{\Omega} \eta(\mathbf{x}^*, t_{m-1}) \xi(\mathbf{x}, t_m) d\mathbf{x} \\ &\quad - \int_{\Omega} \eta(\mathbf{x}, t_m) \xi(\mathbf{x}, t_m) d\mathbf{x} + \Delta t \int_{\Omega} R(\mathbf{x}, t_m) \xi^2(\mathbf{x}, t_m) d\mathbf{x} \\ &\quad + \Delta t \int_{\Omega} R(\mathbf{x}, t_m) \eta(\mathbf{x}, t_m) \xi(\mathbf{x}, t_m) d\mathbf{x} \\ &\quad - \Delta t \int_{\Omega} E_1(c(\mathbf{x}, t_m)) \xi(\mathbf{x}, t_m) d\mathbf{x}. \end{aligned} \quad (3.4)$$

The first term on the right-hand side of Eq. (3.4) is bounded by

$$\begin{aligned} \left| \int_{\Omega} \xi(\mathbf{x}^*, t_{m-1}) \xi(\mathbf{x}, t_m) d\mathbf{x} \right| &\leq \frac{1}{2} \int_{\Omega} \xi^2(\mathbf{x}^*, t_{m-1}) d\mathbf{x} + \frac{1}{2} \int_{\Omega} \xi(\mathbf{x}, t_m) d\mathbf{x} \\ &\leq \frac{1+L\Delta t}{2} \int_{\Omega} \xi^2(\mathbf{x}, t_{m-1}) d\mathbf{x} + \frac{1}{2} \int_{\Omega} \xi(\mathbf{x}, t_m) d\mathbf{x}, \end{aligned} \quad (3.5)$$

where we have used the following relation for the Jacobian determinant

$$\begin{aligned} \det \left(\frac{\partial \mathbf{x}}{\partial \mathbf{x}^*} \right) &= \left[\det \left(\frac{\partial \mathbf{x}^*}{\partial \mathbf{x}} \right) \right]^{-1} \\ &= \left[\det \left(\frac{\partial}{\partial \mathbf{x}} \left[\mathbf{x} - \mathbf{u}(\mathbf{x}, t_m) \Delta t \right] \right) \right]^{-1} = 1 + \mathcal{O}(\Delta t), \end{aligned} \quad (3.6)$$

and have replaced the dummy variable \mathbf{x}^* formally by \mathbf{x} in the first integral on the right-hand side of the last “ \leq ” sign.

The fourth and fifth terms on the right-hand side of Eq. (3.4) are bounded by

$$\begin{aligned} \left| \Delta t \int_{\Omega} R(\mathbf{x}, t_m) \xi^2(\mathbf{x}, t_m) d\mathbf{x} + \Delta t \int_{\Omega} R(\mathbf{x}, t_m) \eta(\mathbf{x}, t_m) \xi(\mathbf{x}, t_m) d\mathbf{x} \right| \\ \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L\Delta t \|\eta(\mathbf{x}, t_m)\|_{L^2}^2 \\ \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L\Delta t h^4 \|c\|_{L^\infty(0,T;H^2)}^2. \end{aligned} \quad (3.7)$$

The last term on the right-hand side of (3.4) was bounded by [7]

$$\begin{aligned} \left| \Delta t \int_{\Omega} E_1(c(\mathbf{x}, t_m)) \xi(\mathbf{x}, t_m) d\mathbf{x} \right| \\ \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L(\Delta t)^2 \left\| \frac{\partial^2 c}{\partial \tau^2} \right\|_{L^2(t_{m-1}, t_m; L^2)}^2. \end{aligned} \quad (3.8)$$

However, the estimate of the remaining two terms on the right-hand side of Eq. (3.4) presents the major difficulty. The techniques used in the previous analyses for the MMOC scheme [4, 7] only lead to a suboptimal-order error estimate that does not reflect the strength of the MMOC and the MMOCAA schemes. To derive an optimal-order error estimate for the MMOC and the MMOCAA schemes, it is crucial to bound these two terms in an optimal order. We present the detailed analyses in the auxiliary lemma in the next section; there we obtain

$$\begin{aligned} \left| \int_{\Omega} \left[\eta(\mathbf{x}, t_m) - \eta(\mathbf{x}^*, t_{m-1}) \right] \xi(\mathbf{x}, t_m) d\mathbf{x} \right| \\ \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L(\Delta t)^3 \|c\|_{L^\infty(0,T;H^2)}^2 \\ + \lambda L\Delta t [h^4 + (\Delta t)^2] \left[\|c\|_{H^1(0,T;H^2)}^2 + \|c\|_{L^\infty(0,T;H^3)}^2 \right], \end{aligned} \quad (3.9)$$

where $\lambda = \text{sgn}(\lfloor Cr \rfloor)$ with Cr being the Courant number defined by

$$Cr = \max_{(\mathbf{x}, t) \in \bar{\Omega} \times [0, T]} \left\{ \frac{|V_1(\mathbf{x}, t)| \Delta t}{\Delta x}, \frac{|V_2(\mathbf{x}, t)| \Delta t}{\Delta y} \right\}. \quad (3.10)$$

Hence, $\lambda = 0$ if $Cr < 1$ and $\lambda = 1$ otherwise.

Incorporating (3.5) through (3.9) into (3.4), we obtain

$$\begin{aligned}
& \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 \\
& \leq \left(\frac{1}{2} + L\Delta t\right) \left[\|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + \|\xi(\mathbf{x}, t_{m-1})\|_{L^2}^2\right] \\
& \quad + L\Delta t[h^4 + (\Delta t)^2]\|c\|_{L^\infty(0,T;H^2)}^2 + L(\Delta t)^2 \left\|\frac{\partial^2 c}{\partial \tau^2}\right\|_{L^2(t_{m-1}, t_m; L^2)}^2 \\
& \quad + \lambda L\Delta t [h^4 + (\Delta t)^2] \left[\|c\|_{H^1(0,T;H^2)}^2 + \|c\|_{L^\infty(0,T;H^3)}^2\right].
\end{aligned} \tag{3.11}$$

Canceling $\frac{1}{2}\|\xi(\mathbf{x}, t_m)\|_{L^2}^2$ on both sides of (3.11) and summing the resulting equation over m , we obtain

$$\begin{aligned}
\|\xi(\mathbf{x}, t_m)\|_{L^2}^2 & \leq L\Delta t \sum_{k=0}^m \|\xi(\mathbf{x}, t_k)\|_{L^2}^2 + L(\Delta t)^2 \left\|\frac{\partial^2 c}{\partial \tau^2}\right\|_{L^2(0,T;L^2)}^2 \\
& \quad + L[h^4 + (\Delta t)^2]\|c\|_{L^\infty(0,T;H^2)}^2 \\
& \quad + \lambda L[h^4 + (\Delta t)^2] \left[\|c\|_{H^1(0,T;H^2)}^2 + \|c\|_{L^\infty(0,T;H^3)}^2\right].
\end{aligned} \tag{3.12}$$

Taking Δt sufficiently small such that $L\Delta t \leq 1/2$ and applying Gronwall's inequality, we obtain the following estimate

$$\begin{aligned}
\|\xi\|_{\dot{L}^\infty(0,T;L^2)} & \leq L[h^2 + \Delta t]\|c\|_{L^\infty(0,T;H^2)} + L\Delta t \left\|\frac{\partial^2 c}{\partial \tau^2}\right\|_{L^2(0,T;L^2)} \\
& \quad + \lambda L [h^2 + \Delta t] \left[\|c\|_{H^1(0,T;H^2)} + \|c\|_{L^\infty(0,T;H^3)}\right].
\end{aligned} \tag{3.13}$$

Combining (3.13) with the estimate (3.2), we obtain

Theorem 3.1. *Let $c(\mathbf{x}, t)$ be the exact solution of (2.1) satisfying $c \in L^\infty(0, T; H^{2+\lambda}(\Omega)) \cap H^1(0, T; H^2(\Omega))$ and $\frac{\partial^2 c}{\partial \tau^2} \in L^2(0, T; H^2(\Omega))$. Let $c_h(\mathbf{x}, t_m)$ be the numerical solution of the MMOC or MMOCOA scheme. Then the following optimal-order L^2 error estimate holds*

$$\begin{aligned}
\|c_h - c\|_{\dot{L}^\infty(0,T;L^2)} & \leq L[h^2 + \Delta t]\|c\|_{L^\infty(0,T;H^2)} + L\Delta t \left\|\frac{\partial^2 c}{\partial \tau^2}\right\|_{L^2(0,T;L^2)} \\
& \quad + \lambda L [h^2 + \Delta t] \left[\|c\|_{H^1(0,T;H^2)} + \|c\|_{L^\infty(0,T;H^3)}\right].
\end{aligned} \tag{3.14}$$

Here $\lambda = 1$ if $Cr < 1$ and 0 otherwise, where the Courant number Cr and λ are defined in (3.10) and below (3.9), respectively.

Remark. *For simplicity of presentation, we have presented the analysis for the MMOC and MMOCOA schemes for two-dimensional advection-reaction equations. The analysis directly carries over to higher-dimensional problem.*

IV. PROOF OF THE AUXILIARY LEMMA

Standard techniques only yield a suboptimal-order estimate

$$\begin{aligned} & \left| \int_{\Omega} \left[\eta(\mathbf{x}, t_m) - \eta(\mathbf{x}^*, t_{m-1}) \right] \xi(\mathbf{x}, t_m) d\mathbf{x} \right| \\ & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L\Delta t h^2 \|c\|_{L^\infty(0,T;H^2)}^2. \end{aligned}$$

This in turn leads to a suboptimal-order estimate of $\mathcal{O}(h + \Delta t)$ for the MMOC and MMOCAA schemes, and does not reflect the strength of these schemes. In this section we prove the following superconvergence estimate

Lemma 4.1. *The following estimate holds*

$$\begin{aligned} & \left| \int_{\Omega} \left[\eta(\mathbf{x}, t_m) - \eta(\mathbf{x}^*, t_{m-1}) \right] \xi(\mathbf{x}, t_m) d\mathbf{x} \right| \\ & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L(\Delta t)^3 \|c\|_{L^\infty(0,T;H^2)}^2 \\ & \quad + \lambda L\Delta t [h^4 + (\Delta t)^2] \left[\|c\|_{H^1(0,T;H^2)}^2 + \|c\|_{L^\infty(0,T;H^3)}^2 \right]. \end{aligned} \quad (4.1)$$

where $\lambda = 1$ for $Cr < 1$ and 0 otherwise.

Proof. Since $Cr \geq 1$ implies $h \geq L\Delta t$, we bound the left-hand side of (4.1) by

$$\begin{aligned} & \left| \int_{\Omega} \left[\eta(\mathbf{x}, t_m) - \eta(\mathbf{x}^*, t_{m-1}) \right] \xi(\mathbf{x}, t_m) d\mathbf{x} \right| \\ & \leq L \|\xi(\mathbf{x}, t_m)\|_{L^2} \left[\|\eta(\mathbf{x}, t_m)\|_{L^2} + \|\eta(\mathbf{x}, t_{m-1})\|_{L^2} \right] \\ & \leq Lh^2 \|\xi(\mathbf{x}, t_m)\|_{L^2} \|c\|_{L^\infty(0,T;H^2)} \\ & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L(\Delta t)^3 \|c\|_{L^\infty(0,T;H^2)}^2. \end{aligned} \quad (4.2)$$

We now concentrate on the case $Cr < 1$. In this case we rewrite the left-hand side of Eq. (4.1) as follows

$$\begin{aligned} & \int_{\Omega} \eta(\mathbf{x}^*, t_{m-1}) \xi(\mathbf{x}, t_m) d\mathbf{x} - \int_{\Omega} \eta(\mathbf{x}, t_m) \xi(\mathbf{x}, t_m) d\mathbf{x} \\ & = - \int_{\Omega} \left[\int_{t_{m-1}}^{t_m} \frac{\partial \eta}{\partial t}(\mathbf{x}, t) dt \right] \xi(\mathbf{x}, t_m) d\mathbf{x} \\ & \quad - \int_{\Omega} \left[\eta(\mathbf{x}, t_{m-1}) - \eta(\mathbf{x}^*, t_{m-1}) \right] \xi(\mathbf{x}, t_m) d\mathbf{x}. \end{aligned} \quad (4.3)$$

The first term on the right-hand side of (4.3) is bounded by

$$\begin{aligned} & \left| \int_{\Omega} \left[\int_{t_{m-1}}^{t_m} \frac{\partial \eta}{\partial t}(\mathbf{x}, t) dt \right] \xi(\mathbf{x}, t_m) d\mathbf{x} \right| \\ & \leq (\Delta t)^{1/2} \int_{\Omega} \left[\int_{t_{m-1}}^{t_m} \left(\frac{\partial \eta}{\partial t}(\mathbf{x}, t) \right)^2 dt \right]^{1/2} |\xi(\mathbf{x}, t_m)| d\mathbf{x} \\ & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L \|\eta\|_{H^1(t_{m-1}, t_m; L^2)}^2 \\ & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + Lh^4 \|c\|_{H^1(t_{m-1}, t_m; H^2)}^2. \end{aligned} \quad (4.4)$$

We now decompose the second term on the right-hand side of Eq. (4.3) as follows

$$\begin{aligned} & \int_{\Omega} \left[\eta(\mathbf{x}, t_{m-1}) - \eta(\mathbf{x}^*, t_{m-1}) \right] \xi(\mathbf{x}, t_m) d\mathbf{x} \\ &= \int_{\Omega} \left[\eta(x, y^*, t_{m-1}) - \eta(x^*, y^*, t_{m-1}) \right] \xi(x, y, t_m) dx dy \\ & \quad + \int_{\Omega} \left[\eta(x, y, t_{m-1}) - \eta(x, y^*, t_{m-1}) \right] \xi(x, y, t_m) dx dy, \end{aligned} \quad (4.5)$$

where

$$x^*(x, y) = x - V_1(x, y, t_m) \Delta t, \quad y^*(x, y) = y - V_2(x, y, t_m) \Delta t. \quad (4.6)$$

We substitute the expression below into the first term on the right-hand side of (4.5)

$$\begin{aligned} & \eta(x, y^*, t_{m-1}) - \eta(x^*, y^*, t_{m-1}) \\ &= \int_0^1 \frac{d}{d\theta} \eta(x^* + \theta(x - x^*), y^*, t_{m-1}) d\theta \\ &= \int_0^1 \frac{\partial \eta}{\partial x} (x^* + \theta(x - x^*), y^*, t_{m-1}) (x - x^*) d\theta, \end{aligned}$$

and then integrate the resulting term by parts to obtain

$$\begin{aligned} & \int_{\Omega} \left[\eta(x, y^*, t_{m-1}) - \eta(x^*, y^*, t_{m-1}) \right] \xi(x, y, t_m) dx dy \\ &= \int_{\Omega} \left[\int_0^1 \frac{\partial \eta}{\partial x} (x^* + \theta(x - x^*), y^*, t_{m-1}) (x - x^*) d\theta \right] \xi(x, y, t_m) dx dy \\ &= - \int_0^1 \int_{\Omega} \left[\frac{\partial \eta}{\partial y} (x^* + \theta(x - x^*), y^*, t_{m-1}) \frac{\partial y^*}{\partial x} (x - x^*) \right. \\ & \quad \left. + \eta(x^* + \theta(x - x^*), y^*, t_{m-1}) \frac{\partial(x - x^*)}{\partial x} \right] \xi(x, y, t_m) dx dy d\theta \\ & \quad - \int_0^1 \int_{\Omega} \eta(x^* + \theta(x - x^*), y^*, t_{m-1}) (x - x^*) \frac{\partial \xi}{\partial x} (x, y, t_m) dx dy d\theta \\ & \quad + \int_0^1 \int_c^d \left\{ \left[\eta(b^* + \theta(b - b^*), y^*, t_{m-1}) (b - b^*) \right] \xi(b, y, t_m) \right. \\ & \quad \left. - \left[\eta(a + \theta(a - a^*), y^*, t_{m-1}) (a - a^*) \right] \xi(a, y, t_m) \right\} dy d\theta. \end{aligned} \quad (4.7)$$

The last term on the right-hand side of (4.7) vanishes due to the periodicity of the functions. Using (4.6) and the fact that

$$\frac{\partial(x - x^*)}{\partial x} = \frac{\partial V_1}{\partial x}(x, y, t_m) \Delta t, \quad \frac{\partial y^*}{\partial x} = -\frac{\partial V_2}{\partial x}(x, y, t_m) \Delta t,$$

we bound the first term on the right-hand side of (4.7) by

$$\begin{aligned} & \left| \int_0^1 \int_{\Omega} \left[\frac{\partial \eta}{\partial y} (x^* + \theta(x - x^*), y^*, t_{m-1}) \frac{\partial y^*}{\partial x} (x - x^*) \right. \right. \\ & \quad \left. \left. + \eta(x^* + \theta(x - x^*), y^*, t_{m-1}) \frac{\partial(x - x^*)}{\partial x} \right] \xi(x, y, t_m) dx dy d\theta \right| \\ & \leq L \Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2} \left[\|\eta(\mathbf{x}, t_{m-1})\|_{L^2} + \Delta t \|\eta(\mathbf{x}, t_m)\|_{H^1} \right] \\ & \leq \Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L \Delta t \left[h^4 + (\Delta t)^2 h^2 \right] \|c\|_{L^\infty(0, T; H^2)}^2. \end{aligned} \quad (4.8)$$

We rewrite the third term on the right-hand side of (4.7) as

$$\begin{aligned}
 & \int_0^1 \int_{\Omega} \eta(x^* + \theta(x - x^*), y^*, t_{m-1})(x - x^*) \frac{\partial \xi}{\partial x}(x, y, t_m) dx dy d\theta \\
 &= \Delta t \int_0^1 \int_{\Omega} \eta(x^* + \theta(x - x^*), y^*, t_{m-1}) V_1(x, y, t_m) \frac{\partial \xi}{\partial x}(x, y, t_m) dx dy d\theta \\
 &= \Delta t \int_{\Omega} V_1(\mathbf{x}, t_m) \frac{\partial \xi}{\partial x}(x, y, t_m) \left[\eta(x, y, t_{m-1}) \right. \\
 &\quad \left. + \int_0^1 \int_0^1 \frac{d}{d\gamma} \eta(x(\gamma, \theta), y(\gamma), t_{m-1}) d\gamma d\theta \right] dx dy \\
 &= \Delta t \int_{\Omega} V_1(\mathbf{x}, t_m) \frac{\partial \xi}{\partial x}(\mathbf{x}, t_m) \eta(\mathbf{x}, t_{m-1}) d\mathbf{x} \\
 &\quad + \Delta t \int_0^1 \int_0^1 \int_{\Omega} V_1(x, y, t_m) \frac{\partial \xi}{\partial x}(x, y, t_m) \\
 &\quad \left[(1 - \theta)(x^* - x) \frac{\partial \eta}{\partial x}(x(\gamma, \theta), y(\gamma), t_{m-1}) \right. \\
 &\quad \left. + (y^* - y) \frac{\partial \eta}{\partial y}(x(\gamma, \theta), y(\gamma), t_{m-1}) \right] dx dy d\gamma d\theta,
 \end{aligned} \tag{4.9}$$

where $x(\gamma, \theta) = x + \gamma(1 - \theta)(x^* - x)$ and $y(\gamma) = y + \gamma(y^* - y)$.

We use the inverse inequality (3.2) to bound the second term on the right-hand side of (4.9)

$$\begin{aligned}
 & \left| \Delta t \int_0^1 \int_0^1 \int_{\Omega} V_1(\mathbf{x}, t_m) \frac{\partial \xi}{\partial x}(\mathbf{x}, t_m) \left[(1 - \theta)(x^* - x) \frac{\partial \eta}{\partial x}(x(\gamma, \theta), y(\gamma), t_{m-1}) \right. \right. \\
 &\quad \left. \left. + (y^* - y) \frac{\partial \eta}{\partial y}(x(\gamma, \theta), y(\gamma), t_{m-1}) \right] d\mathbf{x} d\gamma d\theta \right| \\
 &\leq L(\Delta t)^2 h \|\xi(\mathbf{x}, t_m)\|_{H^1} \|c(\mathbf{x}, t_{m-1})\|_{H^2} \\
 &\leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L(\Delta t)^3 \|c\|_{L^\infty(0, T; H^2)}^2.
 \end{aligned} \tag{4.10}$$

A standard estimate to the first term on the right-hand side of (4.9) yields

$$\begin{aligned}
 & \Delta t \left| \int_{\Omega} V_1(\mathbf{x}, t_m) \eta(\mathbf{x}, t_{m-1}) \frac{\partial \xi}{\partial x}(\mathbf{x}, t_m) d\mathbf{x} \right| \\
 &\leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{H^1} \|c(\mathbf{x}, t_{m-1})\|_{H^2} \\
 &\leq L\Delta t h^2 \|\xi(\mathbf{x}, t_m)\|_{H^1} \|c(\mathbf{x}, t_{m-1})\|_{H^2} \\
 &\leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L\Delta t h^2 \|c(\mathbf{x}, t_{m-1})\|_{H^2}^2,
 \end{aligned} \tag{4.11}$$

where we have used the inverse inequality (3.2) in the last “ \leq ” sign of (4.11). The estimate (4.11) will lead to a suboptimal-order estimate of $\mathcal{O}(h + \Delta t)$ for the MMOC and MMOCOA solutions. To derive an optimal-order estimate for the MMOC and MMOCOA schemes, we have to bound this term in a different way. We sum this term by parts and obtain

$$\begin{aligned}
 & \Delta t \int_{\Omega} V_1(\mathbf{x}, t_m) \eta(\mathbf{x}, t_{m-1}) \frac{\partial \xi}{\partial x}(\mathbf{x}, t_m) d\mathbf{x} \\
 &= \frac{\Delta t}{\Delta x} \sum_{i=1}^I \int_{x_{i-1}}^{x_i} \int_c^d V_1(x, y, t_m) \eta(x, y, t_{m-1}) \left[\xi(x_i, y, t_m) - \xi(x_{i-1}, y, t_m) \right] dx dy =
 \end{aligned}$$

$$\begin{aligned}
&= \frac{\Delta t}{\Delta x} \int_{x_{I-1}}^b \int_c^d V_1(x, y, t_m) \eta(x, y, t_{m-1}) \xi(b, y, t_m) dx dy \\
&\quad - \frac{\Delta t}{\Delta x} \int_a^{x_1} \int_c^d V_1(x, y, t_m) \eta(x, y, t_{m-1}) \xi(a, y, t_m) dx dy \\
&\quad - \frac{\Delta t}{\Delta x} \sum_{i=1}^{I-1} \int_c^d \int_{x_{i-1}}^{x_i} \left[V_1(x + \Delta x, y, t_m) - V_1(x, y, t_m) dz \right] \\
&\quad \quad \eta(x, y, t_{m-1}) \xi(x_i, y, t_m) dx dy \\
&\quad - \frac{\Delta t}{\Delta x} \sum_{i=1}^{I-1} \int_c^d \int_{x_{i-1}}^{x_i} \left[\eta(x + \Delta x, y, t_{m-1}) - \eta(x, y, t_{m-1}) \right] \\
&\quad \quad V_1(x + \Delta x, y, t_m) \xi(x_i, y, t_m) dx dy.
\end{aligned} \tag{4.12}$$

We bound the third term on the right-hand side of (4.12)

$$\begin{aligned}
&\left| \frac{\Delta t}{\Delta x} \sum_{i=1}^{I-1} \int_c^d \int_{x_{i-1}}^{x_i} \left[V_1(x + \Delta x, y, t_m) - V_1(x, y, t_m) \right] \right. \\
&\quad \left. \eta(x, y, t_{m-1}) \xi(x_i, y, t_m) dx dy \right| \\
&\leq L \Delta t \sum_{i=1}^{I-1} \int_c^d \int_{x_{i-1}}^{x_i} \left| \eta(x, y, t_{m-1}) \xi(x_i, y, t_m) \right| dx \\
&\leq L \Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2} \|\eta(\mathbf{x}, t_{m-1})\|_{L^2} \\
&\leq L \Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L \Delta t h^4 \|c\|_{L^\infty(0, T; H^2)}^2,
\end{aligned} \tag{4.13}$$

where in the second “ \leq ” sign, we have used the equivalence between the discrete and continuous L^2 norms. Namely, there are two positive constants L_1 and L_2 such that

$$L_1 \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 \leq \sum_{i=1}^I \Delta x \int_c^d \xi^2(x_i, y, t_m) dy \leq L_2 \|\xi(\mathbf{x}, t_m)\|_{L^2}^2.$$

However, if we similarly bound the last term on the right-hand of Eq. (4.12), we can only obtain a suboptimal-estimate. To derive an optima-order estimate, we introduce a new function $\psi(x, y, t)$ by

$$\psi(x, y, t) = c(x + \Delta x, y, t) - c(x, y, t) = \int_0^{\Delta x} \frac{\partial c}{\partial \alpha}(\alpha + x, y, t) d\alpha. \tag{4.14}$$

Because the spatial partition (2.6) is uniform and $\eta(x + \Delta x, y, t_{m-1})$ is a shift of $c(x, y, t_{m-1})$ by one grid point, so the forward difference operator and the shift operator is commutative. Hence, we have

$$\begin{aligned}
&\eta(x + \Delta x, y, t_{m-1}) - \eta(x, y, t_{m-1}) \\
&= (\Pi - \mathbf{I})c(x + \Delta x, y, t_{m-1}) - (\Pi - \mathbf{I})c(x, y, t_{m-1}) \\
&= (\Pi - \mathbf{I}) \left[c(x + \Delta x, y, t_{m-1}) - c(x, y, t_{m-1}) \right] \\
&= (\Pi - \mathbf{I})\psi(x, y, t_{m-1}).
\end{aligned} \tag{4.15}$$

We substitute the identity (4.15) into the last term on the right-hand side of (4.12) to obtain

$$\begin{aligned}
 & \left| \frac{\Delta t}{\Delta x} \sum_{i=1}^{I-1} \int_c^d \int_{x_{i-1}}^{x_i} \left[\eta(x + \Delta x, y, t_m) - \eta(x, y, t_m) \right] \right. \\
 & \quad \left. + V_1(x + \Delta x, y, t_m) \xi(x_i, y, t_m) dx dy \right| \\
 & \leq \frac{L\Delta t}{\Delta x} \|\xi(\mathbf{x}, t_m)\|_{L^2} \left[\sum_{i=1}^{I-1} \sum_{j=1}^J \int_{y_{j-1}}^{y_j} \int_{x_{i-1}}^{x_i} [(\Pi - \mathbb{I})\psi(\mathbf{x}, t_{m-1})]^2 dx \right]^{1/2} \quad (4.16) \\
 & \leq L\Delta t h \|\xi(\mathbf{x}, t_m)\|_{L^2} \|\psi(\mathbf{x}, t_{m-1})\|_{H^2} \\
 & \leq L\Delta t h^2 \|\xi(\mathbf{x}, t_m)\|_{L^2} \|c(\mathbf{x}, t_{m-1})\|_{H^3}^2 \\
 & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L\Delta t h^4 \|c\|_{L^\infty(0,T;H^3)}^2,
 \end{aligned}$$

where at the last “ \leq ” sign, we have used the inverse inequality (3.2).

We utilize the periodicity of the data to rewrite the first two terms on the right-hand side of Eq. (4.12) as follows:

$$\begin{aligned}
 & \frac{\Delta t}{\Delta x} \int_{x_{I-1}}^b \int_c^d V_1(x, y, t_m) \eta(x, y, t_{m-1}) \xi(b, y, t_m) dx dy \\
 & \quad - \frac{\Delta t}{\Delta x} \int_a^{x_1} \int_c^d V_1(x, y, t_m) \eta(x, y, t_{m-1}) \xi(a, y, t_m) dx dy \\
 & = \frac{\Delta t}{\Delta x} \int_{x_{-1}}^{x_0} \int_c^d V_1(z, y, t_m) \eta(z, y, t_{m-1}) \xi(a, y, t_m) dz dy \\
 & \quad - \frac{\Delta t}{\Delta x} \int_{x_0}^{x_1} \int_c^d V_1(x, y, t_m) \eta(x, y, t_{m-1}) \xi(a, y, t_m) dx dy \\
 & = -\frac{\Delta t}{\Delta x} \int_{x_0}^{x_1} \int_c^d \left[V_1(x, y, t_m) \eta(x, y, t_{m-1}) \right. \\
 & \quad \left. V_1(x - \Delta x, y, t_m) \eta(x - \Delta x, y, t_{m-1}) \right] \xi(a, y, t_m) dx dy \quad (4.17) \\
 & = -\frac{\Delta t}{\Delta x} \int_{x_0}^{x_1} \int_c^d \left[V_1(x, y, t_m) - V_1(x - \Delta x, y, t_m) \right] \\
 & \quad \eta(x, y, t_{m-1}) \xi(a, y, t_m) dx dy \\
 & \quad - \frac{\Delta t}{\Delta x} \int_{x_0}^{x_1} \int_c^d \left[\eta(x, y, t_{m-1}) - \eta(x - \Delta x, y, t_{m-1}) \right] \\
 & \quad V_1(x - \Delta x, y, t_m) \xi(a, y, t_m) dx dy.
 \end{aligned}$$

The first term on the right-hand side of (4.17) is bounded by

$$\begin{aligned}
 & \left| \frac{\Delta t}{\Delta x} \int_{x_0}^{x_1} \int_c^d \left[V_1(x, y, t_m) - V_1(x - \Delta x, y, t_m) \right] \eta(x, y, t_{m-1}) \xi(a, y, t_m) dx dy \right| \\
 & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2} \|\eta(\mathbf{x}, t_{m-1})\|_{L^2} \quad (4.18) \\
 & \leq L\Delta t h^2 \|\xi(\mathbf{x}, t_m)\|_{L^2} \|c(\mathbf{x}, t_{m-1})\|_{H^2}^2 \\
 & \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L\Delta t h^4 \|c\|_{L^\infty(0,T;H^2)}^2,
 \end{aligned}$$

where at the last “ \leq ” sign we have used (4.14) again.

We use (4.15) to bound the second term on the right-hand side of (4.17) as follows

$$\begin{aligned}
& \left| \frac{\Delta t}{\Delta x} \int_{x_0}^{x_1} \int_c^d \left[\eta(x, y, t_{m-1}) - \eta(x - \Delta x, y, t_{m-1}) \right] \right. \\
& \quad \left. V_1(x - \Delta x, y, t_m) \xi(a, y, t_m) dx dy \right| \\
& \leq \frac{L\Delta t}{\Delta x} \sum_{j=1}^J \int_{y_{j-1}}^{y_j} \int_{x_0}^{x_1} \left| (\Pi - \mathbb{I})\psi(x - \Delta x, y, t_{m-1}) \right| |\xi(a, y, t_m)| dx dy \quad (4.19) \\
& \leq L\Delta t h \|\xi(\mathbf{x}, t_m)\|_{L^2} \|\psi(\mathbf{x}, t_{m-1})\|_{H^2} \\
& \leq L\Delta t h^2 \|\xi(\mathbf{x}, t_m)\|_{L^2} \|c(\mathbf{x}, t_{m-1})\|_{H^3}^2 \\
& \leq L\Delta t \|\xi(\mathbf{x}, t_m)\|_{L^2}^2 + L\Delta t h^4 \|c\|_{L^\infty(0, T; H^3)}^2.
\end{aligned}$$

The estimates (4.17) through (4.19) yield an upper bound for the first two terms on the right-hand side of (4.12). Combining (4.7) through (4.12), we have bounded the first term on the right-hand side of (4.5) by the right-hand side of (4.1). By symmetry, we can bound the second term on the right-hand side of (4.5) in the same way. These estimates, together with (4.3) and (4.4), gives the proof of the lemma. \blacksquare

V. NUMERICAL EXPERIMENTS

In this section we perform numerical experiments to verify the theoretically proven optimal-order L^2 convergence rates. The test example is the transport of a two-dimensional rotating Gaussian pulse. The spatial domain is $\Omega = (-0.5, 0.5) \times (-0.5, 0.5)$, the rotating field is imposed as $V_1(x, y) = -4y$, and $V_2(x, y) = 4x$. The time interval is $[0, T] = [0, \pi/2]$, which is the time period required for one complete rotation. The initial condition $c_0(x, y)$ is given by

$$c_0(x, y) = \exp\left(-\frac{(x - x_c)^2 + (y - y_c)^2}{2\sigma^2}\right), \quad (5.1)$$

where x_c , y_c , and σ are the centered and standard deviations, respectively. The corresponding analytical solution at the final time $T = \pi/2$ is identical to the initial condition.

In the numerical experiments, the data are chosen as follows: $x_c = -0.25$, $y_c = 0$, $\sigma = 0.0447$ which gives $2\sigma^2 = 0.0040$. We use a linear regression to fit the convergence rates and the associated constants in the error estimates

$$\|c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\|_{L^p} \leq L_\alpha h^\alpha + L_\beta (\Delta t)^\beta, \quad p = 1, 2. \quad (5.2)$$

We perform two kinds of computations. The first tests the spatial convergence rates of the MMOC and MMOC AA schemes, where we fix a small time step Δt and compute the convergence rate α with respect to h ; the other tests the temporal convergence rate, where we choose a small grid size h and calculate the convergence rate β with respect to Δt . The results are presented in Tables I through ???. These results show that the MMOC and MMOC AA schemes possess second-order accuracy in space and first-order accuracy in time as predicted by Theorem 1 in Section III.

TABLE I. Spatial convergence rate of the MMOC

Δt	h	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^2}$	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^1}$
$\pi/120$	1/50	3.7113×10^{-3}	7.0073×10^{-4}
$\pi/120$	1/60	2.4237×10^{-3}	4.4737×10^{-4}
$\pi/120$	1/70	1.9341×10^{-3}	3.3212×10^{-4}
$\pi/120$	1/80	1.3087×10^{-3}	2.6142×10^{-4}
		$\alpha = 2.14$	$\alpha = 2.09$

TABLE II. Temporal convergence rate of the MMOC

Δt	h	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^2}$	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^1}$
$\pi/56$	1/80	2.0071×10^{-2}	4.1211×10^{-3}
$\pi/64$	1/80	1.7231×10^{-2}	3.6112×10^{-3}
$\pi/72$	1/80	1.6048×10^{-2}	3.1134×10^{-3}
$\pi/80$	1/80	1.3469×10^{-2}	2.8813×10^{-3}
		$\beta = 1.06$	$\beta = 1.03$

TABLE III. Spatial convergence rate of the MMOCAA

Δt	h	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^2}$	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^1}$
$\pi/120$	1/50	3.3445×10^{-3}	6.3148×10^{-4}
$\pi/120$	1/60	2.1647×10^{-3}	4.0658×10^{-4}
$\pi/120$	1/70	1.7236×10^{-3}	2.9836×10^{-4}
$\pi/120$	1/80	1.1745×10^{-3}	2.3152×10^{-4}
		$\alpha = 2.15$	$\alpha = 2.13$

TABLE IV. Temporal convergence rate of the MMOCAA

Δt	h	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^2}$	$\ c_h(\mathbf{x}, T) - c(\mathbf{x}, T)\ _{L^1}$
$\pi/56$	1/80	1.7451×10^{-2}	3.7213×10^{-3}
$\pi/64$	1/80	1.5014×10^{-2}	3.3189×10^{-3}
$\pi/72$	1/80	1.4417×10^{-2}	2.8145×10^{-3}
$\pi/80$	1/80	1.1778×10^{-2}	2.5816×10^{-3}
		$\beta = 1.02$	$\beta = 1.06$

ACKNOWLEDGMENTS

This research was supported in part by South Carolina Commission on Higher Education Grant SCRIG 13060-GA00, and generous awards from Mobil Technology Company and ExxonMobil Upstream Research Company.

REFERENCES

1. J. Bear, (1979). *Hydraulics of Groundwater*, McGraw-Hill, New York.
2. J.P. Benque and J. Ronat, (1982). Quelques difficultes des modeles numeriques en hydraulique. In Glowinski and Lions, editors, *Computing Methods in Applied Sciences and Engineering*, pages 471–494. North-Holland.
3. P.G. Ciarlet, (1978). *The Finite Element Method for Elliptic Problems*, North-Holland, Amsterdam.
4. C.N. Dawson, T.F. Russell, and M.F. Wheeler, (1989). Some improved error estimates for the modified method of characteristics. *SIAM Numer. Anal.*, 26:1487–1512.
5. J. Douglas, Jr., F. Furtado, and F. Pereira, (1997). On the numerical simulation of waterflooding of heterogeneous petroleum reservoirs. *Comput. Geosciences*, 1:155–190.
6. J. Douglas, Jr., C.-S. Huang, and F. Pereira, (1999). The modified method of characteristics with adjusted advection. *Numer. Math.*, 83:353–369.
7. J. Douglas, Jr. and T.F. Russell, (1982). Numerical methods for convection-dominated diffusion problems based on combining the method of characteristics with finite element or finite difference procedures. *SIAM J. Num. Anal.*, 19:871–885.
8. T.F. Dupont, (1970). Galerkin methods for first-order hyperbolic equations: an example. *SIAM Numer. Anal.*, 10:890–899.
9. R.E. Ewing (ed.), (1984). *The Mathematics of Reservoir Simulation*, in Research Frontiers in Applied Mathematics, 1, SIAM, Philadelphia.
10. R.E. Ewing, T.F. Russell, and M.F. Wheeler, (1983). Simulation of miscible displacement using mixed methods and a modified method of characteristics. *SPE 12241*, 71–81.
11. K.W. Morton, A. Priestley, and E. Süli, (1988). Stability of the Lagrangian-Galerkin method with nonexact integration. *RAIRO Modél. Math. Anal. Numer.*, 22:123–151.
12. O. Pironneau, (1982). On the transport-diffusion algorithm and its application to the Navier-Stokes equations. *Numer. Math.*, 38:309–332.
13. T.F. Russell, (1985). Time-stepping along characteristics with incomplete iterations for a Galerkin approximation of miscible displacement in porous media. *SIAM Numer. Anal.*, 22:970–1013.