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AN OPTIMAL-ORDER ERROR ESTIMATE FOR A FAMILY OF ELLAM-MFEM APPROXIMATIONS TO POROUS MEDIUM FLOW*

HONG WANG[†]

Abstract. Mathematical models used to describe porous medium flow lead to coupled systems of time-dependent nonlinear partial differential equations, which present serious mathematical and numerical difficulties. Standard methods tend to generate numerical solutions with nonphysical oscillations or numerical dispersion along with spurious grid-orientation effect. The ELLAM-MFEM time-stepping procedure, in which an Eulerian–Lagrangian localized adjoint method (ELLAM) is used to solve the transport equation and a mixed finite element method (MFEM) is used for the pressure equation, simulates porous medium flow accurately even if large spatial grids and time steps are used. In this paper we prove an optimal-order error estimate for a family of ELLAM-MFEM approximations.

Key words. advection-diffusion equations, characteristic methods, convergence analysis, error estimates, Eulerian–Lagrangian methods, numerical analysis, porous medium flow, subsurface flow

AMS subject classifications. 65M12, 65M15, 65M25, 65M60, 65Z05, 76M10, 76S05

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1. Introduction. Mathematical models used to describe porous medium flow processes in petroleum reservoir simulation, groundwater contaminant transport, and other applications lead to coupled systems of time-dependent nonlinear partial differential equations (PDEs) [2, 11]. Due to the advection-diffusion feature of the transport PDEs, the nonlinearity and couplings of the PDEs in the systems, and the strong effect of sources and sinks, these systems admit solutions with moving steep fronts and complicated structures. Consequently, these problems present serious mathematical and numerical difficulties. Standard finite difference or finite element methods (FDMs and FEMs, respectively) tend to generate solutions with nonphysical oscillations. Upwind methods are often used to stabilize the numerical approximations, but they often produce numerical dispersion and the grid-orientation effect [11]. Extensive research has been carried out on the development of improved methods for advection-diffusion PDEs [16, 18, 21].

An FEM-MFEM time-stepping procedure was presented and analyzed in [8, 9]. In the procedure, a mixed finite element method (MFEM) scheme [4, 5, 20] was used to solve the pressure PDE, and an FEM was used to solve the transport PDE. MFEM schemes generate an accurate approximation to the Darcy velocity, which is required for accurate approximation to the concentration because advection and diffusion dispersion in the transport PDE are governed by Darcy velocity. MFEMs minimize the numerical difficulties occurring in FDMs or FEMs caused by differentiation of the pressure and then multiplication by rough coefficients [22]. Subsequently, an MMOC-MFEM time-stepping procedure was proposed and analyzed in [12, 13], in which the modified method of characteristics (MMOC) [10] was used to replace the FEM scheme in [9]. The MMOC symmetrizes and stabilizes the transport PDE, greatly reduces temporal errors, and so allows for large time steps in a simulation without loss of

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accuracy. However, the MMOC fails to conserve mass and has difficulties in handling general boundary conditions.

The Eulerian–Lagrangian localized adjoint method (ELLAM) framework [6, 21] provides a systematic approach to solve transient advection–diffusion PDEs with general boundary conditions in a mass-conservative manner, while maintaining accuracy and efficiency of Eulerian–Lagrangian methods. Numerical experiments show that the ELLAM is very competitive in the context of model transport PDEs [26, 28] and miscible porous medium flow [3, 17, 30, 32]. Nevertheless, corresponding theoretical analysis falls far behind. To date, error estimates for the ELLAM and related schemes have been proved in the context of linear advection-dominated transport PDEs [1, 14, 15, 24, 25, 27, 29, 31]. This is partly due to the fact that the analyses are more complex than those for the MMOC and related methods [10, 29, 21]. In this paper we derive an optimal-order error estimate for an ELLAM-MFEM approximation to the coupled system of miscible porous medium flow.

The rest of the paper is organized as follows: In section 2 we review the mathematical model. In section 3 we describe the ELLAM-MFEM time-stepping procedure. In section 4 we present known theoretical results used in the analysis. In section 5 we prove an optimal-order error estimate for the ELLAM-MFEM time-stepping procedure. In section 6 we prove several lemmas used in section 5.

2. Mathematical model and notation. We present a mathematical model for porous medium flow and introduce the functional spaces used in this paper.

2.1. Mathematical model. Let $c(\mathbf{x}, t)$ be the concentration of an invading fluid or a concerned solute/solvent, and let $p(\mathbf{x}, t)$ and $\mathbf{u}(\mathbf{x}, t)$ be the pressure and Darcy velocity of the fluid mixture, respectively. The mass conservation for the fluid mixture incorporated with the incompressibility condition, Darcy’s law, and the mass conservation for the invading fluid lead to the following system of PDEs [2, 11]:

$$(2.1) \quad \nabla \cdot \mathbf{u} = q, \quad \mathbf{u} = -\frac{\mathbf{K}}{\mu(c)}(\nabla p - \rho g \nabla d), \quad \mathbf{x} \in \Omega, \quad t \in [0, T],$$

$$(2.2) \quad \phi \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{x}, \mathbf{u})\nabla c) = \bar{c}q, \quad \mathbf{x} \in \Omega, \quad t \in [0, T],$$

$$(2.3) \quad \begin{aligned} \mathbf{u} \cdot \mathbf{n} &= (\mathbf{D}\nabla c) \cdot \mathbf{n} = 0, & \mathbf{x} \in \partial\Omega, \quad t \in [0, T], \\ c(\mathbf{x}, 0) &= c_0(\mathbf{x}), & \mathbf{x} \in \Omega. \end{aligned}$$

We assume that the medium is homogeneous vertically and take $\Omega \subset \mathbb{R}^2$ with a nonuniform local elevation. $\phi(\mathbf{x})$ and $\mathbf{K}(\mathbf{x})$ are the porosity and the permeability tensor of the medium, respectively, $\mu(c)$ and ρ are the viscosity and the density of the fluid mixture, respectively, g is the gravitational acceleration, $d(\mathbf{x})$ is the reservoir depth, and $q(\mathbf{x}, t)$ is the source and sink term. $\mathbf{D}(\mathbf{x}, \mathbf{u}) = \phi(\mathbf{x})d_m \mathbf{I} + d_t|\mathbf{u}| + (d_l - d_t)(u_i u_j)_{i,j=1}^2/|\mathbf{u}|$ is the diffusion-dispersion tensor, with d_m , d_t , and d_l being the molecular diffusion and the transverse and longitudinal dispersivities, respectively, and \mathbf{I} is the identity tensor. $\bar{c}(\mathbf{x}, t)$ is specified at sources and $\bar{c}(\mathbf{x}, t) = c(\mathbf{x}, t)$ at sinks. $c_0(\mathbf{x})$ is the initial concentration.

The combination of the first equations in (2.1) and (2.3) implies that q has mean 0. In addition, (2.1) with the noflow boundary condition (2.3) can determine the pressure $p(\mathbf{x}, t)$ only up to an additive constant for all the time $t \in [0, T]$. But this indeterminacy is of no consequence since \mathbf{u} is uniquely determined by Darcy’s law, and only \mathbf{u} (not p) is needed in (2.2).

2.2. Notation. Let $W_q^m(\Omega)$ be the Sobolev spaces consisting of functions whose derivatives up to order- m are q th integrable on Ω , and $H^m(\Omega) := W_2^m(\Omega)$. Let $L_0^2(\Omega)$ be the subspace of $L^2(\Omega)$ with mean 0. We introduce vector-valued Sobolev spaces

$$\begin{aligned} H^m(\text{div}; \Omega) &:= \left\{ \mathbf{f}(\mathbf{x}) = (f_1, f_2) : f_1, f_2, \nabla \cdot \mathbf{f} \in H^m(\Omega) \right\}, \\ \|\mathbf{f}\|_{H^m(\text{div}; \Omega)} &:= \left(\|f_1\|_{H^m(\Omega)}^2 + \|f_2\|_{H^m(\Omega)}^2 + \|\nabla \cdot \mathbf{f}\|_{H^m(\Omega)}^2 \right)^{1/2}, \\ H_0(\text{div}; \Omega) &:= \left\{ \mathbf{f}(\mathbf{x}) \in H^0(\text{div}; \Omega) : \mathbf{f}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = 0, \mathbf{x} \in \partial\Omega \right\}. \end{aligned}$$

We drop Ω in these notations when it is clear from the context.

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

$$\begin{aligned} W_q^m(t_1, t_2; X) &:= \left\{ f(\mathbf{x}, t) : \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X \in L^q(t_1, t_2), 0 \leq \alpha \leq m, 1 \leq q \leq \infty \right\}, \\ \|f\|_{W_q^m(t_1, t_2; X)} &:= \begin{cases} \left(\sum_{\alpha=0}^m \int_{t_1}^{t_2} \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X^q dt \right)^{1/q}, & 1 \leq q < \infty, \\ \max_{0 \leq \alpha \leq m} \text{esssup}_{t \in (t_1, t_2)} \left\| \frac{\partial^\alpha f}{\partial t^\alpha}(\cdot, t) \right\|_X, & q = \infty. \end{cases} \end{aligned}$$

We also define the discrete norms

$$\begin{aligned} \|f\|_{\hat{L}_c^\infty(0, T; X)} &:= \max_{0 \leq n \leq N} \|f(\mathbf{x}, t_n^c)\|_X, & \|f\|_{\hat{L}_p^\infty(0, T; X)} &:= \max_{0 \leq m \leq M} \|f(\mathbf{x}, t_m^p)\|_X, \\ \|f\|_{\hat{L}_c^2(0, T; X)} &:= \left(\sum_{n=0}^N \|f(\mathbf{x}, t_n^c)\|_X^2 \Delta t_n^c \right)^{1/2}, \end{aligned}$$

with t_n^c and t_m^p being defined in (3.1) and (3.11), respectively. If $(t_1, t_2) = (0, T)$, we drop it from these notations.

In this paper we use ε to denote an arbitrarily small positive number, A_i , K_i , and Q_i to denote fixed positive constants, and Q to denote a generic positive constant that could assume different values at different occurrences. All of these constants are independent of spatial and temporal grid parameters.

3. An ELLAM-MFEM time-stepping procedure. In this procedure an ELLAM scheme is used to solve the transport PDE (2.2), and an MFEM scheme is used for the pressure system (2.1).

3.1. An ELLAM formulation for the transport equation. We define a temporal partition on the interval $[0, T]$ by

$$(3.1) \quad 0 =: t_0^c < t_1^c < \dots < t_n^c < \dots < t_{N-1}^c < t_N^c := T,$$

with $\Delta t_n^c := t_n^c - t_{n-1}^c$ and $\Delta t_c := \max_{1 \leq n \leq N} \Delta t_n^c$.

By multiplying (2.2) by any space-time test functions z that are continuous and piecewise smooth, vanish outside the space-time strip $\Omega \times (t_{n-1}^c, t_n^c]$, and are discon-

tinuous in time at time t_{n-1}^c , we obtain a weak formulation for (2.2)

$$\begin{aligned}
 (3.2) \quad & \int_{\Omega} \phi(\mathbf{x}) c(\mathbf{x}, t_n^c) z(\mathbf{x}, t_n^c) d\mathbf{x} + \int_{t_{n-1}^c}^{t_n^c} \int_{\Omega} \nabla z(\mathbf{y}, \theta) \cdot \mathbf{D}(\mathbf{y}, \mathbf{u}(\mathbf{y}, \theta)) \nabla c(\mathbf{y}, \theta) d\mathbf{y} d\theta \\
 & - \int_{t_{n-1}^c}^{t_n^c} \int_{\Omega} c(\mathbf{y}, \theta) \left[\phi(\mathbf{y}) \frac{\partial z(\mathbf{y}, \theta)}{\partial \theta} + \mathbf{u}(\mathbf{y}, \theta) \cdot \nabla z(\mathbf{y}, \theta) \right] d\mathbf{y} d\theta \\
 & = \int_{\Omega} \phi(\mathbf{x}) c(\mathbf{x}, t_{n-1}^c) z(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} + \int_{t_{n-1}^c}^{t_n^c} \int_{\Omega} \bar{c}(\mathbf{y}, \theta) q(\mathbf{y}, \theta) z(\mathbf{y}, \theta) d\mathbf{y} d\theta,
 \end{aligned}$$

where $z(\mathbf{x}, t_{n-1}^{c,+}) := \lim_{t \rightarrow t_{n-1}^c, t > t_{n-1}^c} z(\mathbf{x}, t)$ accounts for the discontinuity of $z(\mathbf{x}, t)$ in time at time t_{n-1}^c . We replace the dummy variables \mathbf{x} and t in the space-time integrals in (3.2) by \mathbf{y} and θ and reserve \mathbf{x} for the point in Ω at time t_n^c or t_{n-1}^c .

In the ELLAM framework [6, 21, 30], the test functions in (3.2) are defined to be the solutions of the adjoint equation of the hyperbolic part of (2.2)

$$(3.3) \quad \phi(\mathbf{y}) \frac{\partial z(\mathbf{y}, \theta)}{\partial \theta} + \mathbf{u}(\mathbf{y}, \theta) \cdot \nabla z(\mathbf{y}, \theta) = 0, \quad \mathbf{y} \in \bar{\Omega}, \quad \theta \in [t_{n-1}^c, t_n^c].$$

Thus, the last term on the left-hand side of (3.2) vanishes. Once the test functions $z(\mathbf{x}, t_n^c)$ are specified in Ω , they are determined in the space-time strip $\Omega \times (t_{n-1}^c, t_n^c]$ by constant extension along the characteristics $\mathbf{y} = \mathbf{r}(\theta; \mathbf{x}, t_n^c)$ defined by

$$(3.4) \quad \frac{d\mathbf{r}}{d\theta} = \frac{\mathbf{u}(\mathbf{r}, \theta)}{\phi(\mathbf{r})} \quad \text{and} \quad \mathbf{r}(\theta; \bar{\mathbf{x}}, \bar{t}) \Big|_{\theta=\bar{t}} = \bar{\mathbf{x}}.$$

Evaluating the source term in (3.2) by the Euler formula at time t_n^c yields

$$\begin{aligned}
 (3.5) \quad & \int_{t_{n-1}^c}^{t_n^c} \int_{\Omega} \bar{c}(\mathbf{y}, \theta) q(\mathbf{y}, \theta) z(\mathbf{y}, \theta) d\mathbf{y} d\theta \\
 & = \int_{\Omega} \int_{t_{n-1}^c}^{t_n^c} \bar{c}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) q(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) z(\mathbf{x}, t_n^c) \det \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right) d\theta d\mathbf{x} \\
 & = \Delta t_n^c \int_{\Omega} \bar{c}(\mathbf{x}, t_n^c) q(\mathbf{x}, t_n^c) z(\mathbf{x}, t_n^c) d\mathbf{x} + E_q(\bar{c}, z),
 \end{aligned}$$

where $E_q(\bar{c}, z)$ is the local truncation error term given by

$$\begin{aligned}
 (3.6) \quad E_q(\bar{c}, z) := & - \int_{\Omega} z(\mathbf{x}, t_n^c) \left\{ \int_{t_{n-1}^c}^{t_n^c} \left[\bar{c}(\mathbf{x}, t_n^c) q(\mathbf{x}, t_n^c) \right. \right. \\
 & \left. \left. - \bar{c}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) q(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) \det \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right) \right] d\theta \right\} d\mathbf{x}.
 \end{aligned}$$

In (3.5) we have implicitly used the fact that the traceback operator \mathbf{r} is a diffeomorphism and the determinant is positive [10].

Likewise, we evaluate the diffusion-dispersion term in (3.2) to obtain

$$\begin{aligned}
 & \int_{t_{n-1}^c}^{t_n^c} \int_{\Omega} \nabla z(\mathbf{y}, \theta) \cdot \mathbf{D}(\mathbf{y}, \mathbf{u}(\mathbf{y}, \theta)) \nabla c(\mathbf{y}, \theta) d\mathbf{y} d\theta \\
 &= \int_{\Omega} \int_{t_{n-1}^c}^{t_n^c} \nabla_{\mathbf{r}} z(\mathbf{x}, t_n^c) \cdot (\mathbf{D}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta))) \\
 & \quad \nabla c_{\mathbf{r}}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) \det \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right) d\theta d\mathbf{x} \\
 (3.7) \quad &= \int_{\Omega} \int_{t_{n-1}^c}^{t_n^c} \det \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right) \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right)^{-1} \nabla z(\mathbf{x}, t_n^c) \\
 & \quad \cdot (\mathbf{D}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta))) \nabla c_{\mathbf{r}}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) d\theta d\mathbf{x} \\
 &= \Delta t_n^c \int_{\Omega} \nabla z(\mathbf{x}, t_n^c) \cdot \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c)) \nabla c(\mathbf{x}, t_n^c) d\mathbf{x} + E_{\mathbf{D}}(c, z).
 \end{aligned}$$

The subscript \mathbf{r} emphasizes that the gradient is taken with respect to \mathbf{r} . The local truncation error $E_{\mathbf{D}}(c, z)$ is given by

$$\begin{aligned}
 E_{\mathbf{D}}(c, z) &:= \int_{\Omega} \int_{t_{n-1}^c}^{t_n^c} \left(\det \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right) \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right)^{-1} - \mathbf{I} \right) \nabla z(\mathbf{x}, t_n^c) \\
 (3.8) \quad & \quad \cdot (\mathbf{D}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta))) \nabla c(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) d\theta d\mathbf{x} \\
 & - \int_{\Omega} \int_{t_{n-1}^c}^{t_n^c} \nabla z(\mathbf{x}, t_n) \cdot (\mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c))) \nabla c(\mathbf{x}, t_n^c) \\
 & \quad - \mathbf{D}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta)) \nabla c(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) d\theta d\mathbf{x}.
 \end{aligned}$$

We substitute (3.5) and (3.7) into (3.2) to obtain an ELLAM reference equation for the transport PDE (2.2)

$$\begin{aligned}
 & \int_{\Omega} \phi(\mathbf{x}) c(\mathbf{x}, t_n^c) z(\mathbf{x}, t_n^c) d\mathbf{x} + \Delta t_n^c \int_{\Omega} \nabla z(\mathbf{x}, t_n^c) \cdot \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c)) \nabla c(\mathbf{x}, t_n^c) d\mathbf{x} \\
 (3.9) \quad &= \int_{\Omega} \phi(\mathbf{x}) c(\mathbf{x}, t_{n-1}^c) z(\mathbf{x}, t_{n-1}^c) d\mathbf{x} + \Delta t_n^c \int_{\Omega} \bar{c}(\mathbf{x}, t_n^c) q(\mathbf{x}, t_n^c) z(\mathbf{x}, t_n^c) d\mathbf{x} \\
 & - E_{\mathbf{D}}(c, z) + E_q(\bar{c}, z).
 \end{aligned}$$

3.2. An MFEM formulation for the pressure and Darcy velocity. We multiply the second equation in (2.1) by $\mu(c)\mathbf{K}^{-1}(\mathbf{x})$ and any test functions $\mathbf{v} \in H_0(\text{div}; \Omega)$ and apply the divergence theorem to the ∇p term. We then multiply the first equation in (2.1) by any test functions $w(\mathbf{x}) \in L_0^2(\Omega)$ and integrate over Ω . The system (2.1) is expressed as a time-parameterized saddle-point problem of finding a map $(\mathbf{u}(\mathbf{x}, t), p(\mathbf{x}, t)) \in H_0(\text{div}; \Omega) \times L_0^2(\Omega)$ such that

$$\begin{aligned}
 & \int_{\Omega} \mu(c)\mathbf{K}^{-1}\mathbf{u} \cdot \mathbf{v} d\mathbf{x} - \int_{\Omega} p \nabla \cdot \mathbf{v} d\mathbf{x} = \int_{\Omega} \rho g \nabla d \cdot \mathbf{v} d\mathbf{x}, \\
 (3.10) \quad & \int_{\Omega} w \nabla \cdot \mathbf{u} d\mathbf{x} = \int_{\Omega} q(\mathbf{x}, t) w d\mathbf{x} \\
 & \forall (\mathbf{v}(\mathbf{x}), w(\mathbf{x})) \in H_0(\text{div}; \Omega) \times L_0^2(\Omega), t \in [0, T].
 \end{aligned}$$

It was proved [4, 8] that problem (3.10) has a unique solution $(\mathbf{u}(\mathbf{x}, t), p(\mathbf{x}, t)) \in H_0(\text{div}; \Omega) \times L_0^2(\Omega)$ for all $t \in [0, T]$.

Let $V^k \subset H_0(\text{div}; \Omega)$ and $S_p^k \subset L_0^2(\Omega)$ be MFEM spaces of index $k \geq 0$ on a quasi-uniform partition of $\Omega = \cup \Omega_e^p$ with the diameter h_p [5, 20]. We define a temporal partition on the time interval $[0, T]$ for the pressure grid by

$$(3.11) \quad 0 =: t_0^p < t_1^p < \cdots < t_m^p < \cdots < t_{M-1}^p < t_M^p := T,$$

with $\Delta t_m^p := t_m^p - t_{m-1}^p$ and $\Delta t_p := \max_{1 \leq m \leq M} \Delta t_m^p$.

Given a concentration approximation $c_h(\mathbf{x}, t_m^p)$ at time t_m^p , the MFEM scheme determines the velocity $\mathbf{u}_h(\mathbf{x}, t_m^p) \in V^k$ and the pressure $p_h(\mathbf{x}, t_m^p) \in S_p^k$ such that

$$(3.12) \quad \begin{aligned} & \int_{\Omega} \mu(c_h(\mathbf{x}, t_m^p)) \mathbf{K}^{-1}(\mathbf{x}) \mathbf{u}_h(\mathbf{x}, t_m^p) \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x} - \int_{\Omega} p_h(\mathbf{x}, t_m^p) \nabla \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x} \\ & = \int_{\Omega} \rho g \nabla d(\mathbf{x}) \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x} \quad \forall \mathbf{v}_h(\mathbf{x}) \in V^k, \\ & \int_{\Omega} w_h(\mathbf{x}) \nabla \cdot \mathbf{u}_h(\mathbf{x}, t_m^p) d\mathbf{x} = \int_{\Omega} q(\mathbf{x}, t_m^p) w_h(\mathbf{x}) d\mathbf{x} \quad \forall w_h(\mathbf{x}) \in S_p^k. \end{aligned}$$

3.3. An ELLAM-MFEM time-stepping procedure. The velocity field usually changes less rapidly than the concentration. Moreover, at each time step the MFEM system (3.12) is more expensive to solve than the ELLAM scheme for the transport PDE (2.2). Therefore, we allow a larger time step for the pressure than that for the concentration [9]. It is often computationally convenient to define the time partition (3.1) for the concentration by subdividing the time partition (3.11) for the pressure. Namely, there exist $0 =: N_0 < N_1 < \cdots < N_m < \cdots < N_{M-1} < N_M := N$ such that $t_{N_m}^c = t_m^p$ for $m = 1, 2, \dots, M$. For $n = N_{m-1} + 1, N_{m-1} + 2, \dots, N_m$, the concentration time step t_n^c relates to the pressure time steps by $t_{m-1}^p < t_n^c \leq t_m^p$. In the ELLAM scheme we define a velocity approximation $\mathbf{u}_h^E(\mathbf{x}, t_n^c)$ by an extrapolation of $\mathbf{u}_h(\mathbf{x}, t_{m-1}^p)$ and earlier values [9]

$$(3.13) \quad \mathbf{u}_h^E(\mathbf{x}, t_n^c) := \begin{cases} \left(1 + \frac{t_n^c - t_{m-1}^p}{\Delta t_{m-1}^p} \right) \mathbf{u}_h(\mathbf{x}, t_{m-1}^p) - \frac{t_n^c - t_{m-1}^p}{\Delta t_{m-1}^p} \mathbf{u}_h(\mathbf{x}, t_{m-2}^p), \\ \quad N_{m-1} + 1 \leq n \leq N_m, \quad 2 \leq m \leq M, \\ \mathbf{u}_h(\mathbf{x}, 0), \quad 1 \leq n \leq N_1, \quad m = 1. \end{cases}$$

Let $S_c^l \subset W_{\infty}^1(\Omega)$ be an FEM space, which contains the space of continuous piecewise polynomials of degree at most l on a quasi-uniform partition of diameter h_c . For example, the FEM space S_c^l could be the space of piecewise polynomials of degree at most l on triangular elements or the space of piecewise polynomials of degree at most l in each coordinate direction on rectangular elements. We often utilize the fact that velocity is smoother than the concentration to use a much larger grid size h_p than h_c and to further reduce computational cost since (3.12) is more expensive to solve than (3.14).

Let $c_h(\mathbf{x}, 0)$ be an approximation to $c_0(\mathbf{x})$ (e.g., its L^2 or Ritz projection, or interpolation). An ELLAM-MFEM time-stepping procedure is formulated as follows: For $m = 1, \dots, M$, solve the MFEM scheme (3.12) at the pressure time step t_{m-1}^p . For $n = N_{m-1} + 1, N_{m-1} + 2, \dots, N_m$, solve the following ELLAM scheme at each

concentration time step t_n^c : Find $c_h(\mathbf{x}, t_n^c) \in S_c^l$ such that for all $z_h(\mathbf{x}, t_n^c) \in S_c^l$

$$\begin{aligned}
 & \int_{\Omega} \phi(\mathbf{x}) c_h(\mathbf{x}, t_n^c) z_h(\mathbf{x}, t_n^c) d\mathbf{x} \\
 (3.14) \quad & + \Delta t_n^c \int_{\Omega} \nabla z_h(\mathbf{x}, t_n^c) \cdot \mathbf{D}(\mathbf{x}, \mathbf{u}_h^E(\mathbf{x}, t_n^c)) \nabla c_h(\mathbf{x}, t_n^c) d\mathbf{x} \\
 & = \int_{\Omega} \phi(\mathbf{x}) c_h(\mathbf{x}, t_{n-1}^c) z_h(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} + \Delta t_n^c \int_{\Omega} \bar{c}_h(\mathbf{x}, t_n^c) q(\mathbf{x}, t_n^c) z_h(\mathbf{x}, t_n^c) d\mathbf{x}.
 \end{aligned}$$

All of the integrals in (3.14), except for the first on the right-hand side, are in Eulerian coordinates and can be evaluated as in FEMs. The first term on the right-hand side of (3.14) is in Lagrangian coordinates and requires extra attention. By definition, the test functions z in the ELLAM reference equation (3.9) are constant along the characteristics \mathbf{r} defined by the initial-value problem (3.4). Set

$$(3.15) \quad \tilde{\mathbf{x}} := \mathbf{r}(t_n^c; \mathbf{x}, t_{n-1}^c) = \mathbf{x} + \int_{t_{n-1}^c}^{t_n^c} \frac{\mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c), \theta)}{\phi(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c))} d\theta;$$

the test function $z(\mathbf{x}, t_{n-1}^c)$ in (3.9) is determined by

$$(3.16) \quad z(\mathbf{x}, t_{n-1}^{c,+}) = z(\tilde{\mathbf{x}}, t_n^c).$$

Unlike in linear advection-diffusion PDEs [6, 26], the velocity \mathbf{u} is unknown. In (3.14) we compute an approximate characteristic $\mathbf{r}_h(t_n^c; \mathbf{x}, t_{n-1}^c)$ by solving a numerical analogue of problem (3.4)

$$(3.17) \quad \frac{d\mathbf{r}_h}{d\theta} = \frac{\mathbf{u}_h^E(\mathbf{r}_h, \theta)}{\phi(\mathbf{r}_h)} \quad \text{and} \quad \mathbf{r}_h(\theta; \bar{\mathbf{x}}, \bar{t}) \Big|_{\theta=\bar{t}} = \bar{\mathbf{x}}.$$

For clarity of exposition, we assume an Euler tracking and set

$$\begin{aligned}
 (3.18) \quad \tilde{\mathbf{x}}_h & := \mathbf{r}_h(t_n^c; \mathbf{x}, t_{n-1}^c) = \mathbf{x} + \int_{t_{n-1}^c}^{t_n^c} \frac{\mathbf{u}_h^E(\mathbf{r}_h(\theta; \mathbf{x}, t_{n-1}^c), \theta)}{\phi(\mathbf{r}_h(\theta; \mathbf{x}, t_{n-1}^c))} d\theta \\
 & = \mathbf{x} + \frac{\mathbf{u}_h^E(\mathbf{x}, t_{n-1}^c)}{\phi(\mathbf{x})} \Delta t_n^c.
 \end{aligned}$$

The test functions $z_h(\mathbf{x}, t_{n-1}^c)$ in the ELLAM scheme (3.14) are evaluated by

$$(3.19) \quad z_h(\mathbf{x}, t_{n-1}^{c,+}) = z_h(\tilde{\mathbf{x}}_h, t_n^c).$$

This further complicates the analysis for the ELLAM-MFEM procedure.

4. Preliminaries. This section cites well-established estimates to be used in the proof of the main theorem in section 5.

The finite element space S_c^l has the approximation and inverse properties [7] for $1 \leq m \leq l + 1, 1 \leq p, q \leq \infty$

$$(4.1) \quad \inf_{z_h \in S_c^l} (\|z - z_h\|_{L^q} + h_c \|z - z_h\|_{W_q^1}) \leq A_1 h_c^{m+1+(\frac{2}{q}-\frac{2}{p})} \|z\|_{W_p^m} \quad \forall z \in W_p^m(\Omega)$$

and

$$\begin{aligned}
 (4.2) \quad & \|z_h\|_{H^1} \leq K_1 h_c^{-1} \|z_h\|_{L^2}, \quad \|z_h\|_{L^\infty} \leq K_1 |\ln h_c|^{1/2} \|z_h\|_{H^1}, \\
 & \|z_h\|_{W_q^m} \leq K_1 h_c^{-(1-\frac{2}{q})} \|z_h\|_{H^m} \quad \forall z_h \in S_c^l, \quad m = 0, 1.
 \end{aligned}$$

The MFEM spaces (V^k, S_p^k) have the approximation and inverse properties [4, 5, 7, 19] for $2 \leq q \leq +\infty$ and $1 \leq m \leq k + 1$

$$(4.3) \quad \begin{aligned} \inf_{\mathbf{v}_h \in V^k} \|\mathbf{v} - \mathbf{v}_h\|_{L^q} &\leq A_2 h_p^{m-(1-\frac{2}{q})} \|\mathbf{v}\|_{H^m} \quad \forall \mathbf{v} \in H^m, \\ \inf_{\mathbf{v}_h \in V^k} \|\mathbf{v} - \mathbf{v}_h\|_{H(\text{div})} &\leq A_2 h_p^m \|\mathbf{v}\|_{H^m(\text{div})} \quad \forall \mathbf{v} \in H^m(\text{div}), \\ \inf_{g_h \in S_p^k} \|g - g_h\|_{L^2} &\leq A_2 h_p^m \|g\|_{H^m} \quad \forall g \in H^m \end{aligned}$$

and

$$(4.4) \quad \begin{aligned} \|\mathbf{v}_h\|_{L^q} &\leq K_2 h_p^{-(1-\frac{2}{q})} \|\mathbf{v}_h\|_{L^2} \quad \forall \mathbf{v}_h \in V^k, \\ \|\mathbf{v}_h\|_{W_q^1} &\leq K_2 h_p^{-1} \|\mathbf{v}_h\|_{L^q} \quad \forall \mathbf{v}_h \in V^k. \end{aligned}$$

It is understood in (4.4) that

$$\|\mathbf{v}_h\|_{W_q^1} := \begin{cases} \left(\sum_{\Omega_e^p \subset \Omega} \|\mathbf{v}_h\|_{W_q^1(\Omega_e^p)}^q \right)^{1/q} & \text{for } 2 \leq q < +\infty, \\ \max_{\forall \Omega_e^p \subset \Omega} \|\mathbf{v}_h\|_{W_q^1(\Omega_e^p)} & \text{for } q = +\infty, \end{cases}$$

where $\Omega_e^p \subset \Omega$ are all of the elements of the pressure mesh.

Let $\Pi c(\mathbf{x}, t) \in S_c^l$, $t \in [0, T]$, be the Ritz projection of $c(\mathbf{x}, t)$ defined by [23, 33]

$$(4.5) \quad \begin{aligned} \int_{\Omega} \chi(\mathbf{x})(\Pi c(\mathbf{x}, t) - c(\mathbf{x}, t)) d\mathbf{x} \\ + \int_{\Omega} \nabla \chi(\mathbf{x}) \cdot \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t)) \nabla(\Pi c(\mathbf{x}, t) - c(\mathbf{x}, t)) d\mathbf{x} = 0 \quad \forall \chi \in S_c^l. \end{aligned}$$

The following estimates hold [7, 19, 23, 33] for $2 \leq q \leq +\infty$, $1 \leq m \leq l + 1$:

$$(4.6) \quad \begin{aligned} \|\Pi c - c\|_{L^\infty(L^q)} + h_c \|\Pi c - c\|_{L^\infty(W_q^1)} &\leq A_1 h_c^m \|c\|_{L^\infty(W_q^m)}, \\ \|\Pi c - c\|_{H^1(L^q)} &\leq A_1 h_c^m \|c\|_{H^1(W_q^m)}. \end{aligned}$$

Here the constant A_1 is independent of c and h_c .

Let $\mathbf{I}c(\mathbf{x}, t) \in S_c^l$, $t \in [0, T]$, be the interpolation of $c(\mathbf{x}, t)$. We use the estimates (4.1) with $p = 2$ and $q = +\infty$, (4.2) with $q = +\infty$, and (4.6) with $q = 2$ to conclude that for $c \in L^\infty(W_\infty^1 \cap H^2)$

$$(4.7) \quad \begin{aligned} \|\Pi c\|_{L^\infty(W_\infty^1)} &\leq \|\Pi c - \mathbf{I}c\|_{L^\infty(W_\infty^1)} + \|\mathbf{I}c - c\|_{L^\infty(W_\infty^1)} + \|c\|_{L^\infty(W_\infty^1)} \\ &\leq K_1 h_c^{-1} \|\Pi c - \mathbf{I}c\|_{L^\infty(H^1)} + (A_1 + 1) \|c\|_{L^\infty(W_\infty^1)} \\ &\leq K_1 h_c^{-1} (\|\Pi c - c\|_{L^\infty(H^1)} + \|\mathbf{I}c - c\|_{L^\infty(H^1)}) \\ &\quad + (A_1 + 1) \|c\|_{L^\infty(W_\infty^1)} \\ &\leq 2A_1 K_1 \|c\|_{L^\infty(H^2)} + (A_1 + 1) \|c\|_{L^\infty(W_\infty^1)} =: K_3. \end{aligned}$$

We similarly define a mapping $(\Pi\mathbf{u}, \Pi p)$ from $H(\text{div}) \times L_0^2$ to $V^k \times S_p^k$ by

$$(4.8) \quad \begin{aligned} & \int_{\Omega} \mu(c(\mathbf{x}, t)) \mathbf{K}^{-1}(\mathbf{x}) (\Pi\mathbf{u}(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, t)) \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x} \\ & - \int_{\Omega} (\Pi p(\mathbf{x}, t) - p(\mathbf{x}, t)) \nabla \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x} = 0 \quad \forall \mathbf{v}_h \in V^k, \\ & \int_{\Omega} w_h(\mathbf{x}) \nabla \cdot (\Pi\mathbf{u}(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, t)) d\mathbf{x} = 0 \quad \forall w_h \in S_p^k. \end{aligned}$$

The following estimates hold, e.g., for Raviart–Thomas spaces [4, 8, 9]:

$$(4.9) \quad \begin{aligned} & \|\Pi\mathbf{u} - \mathbf{u}\|_{L^\infty(H(\text{div}))} + \|\Pi p - p\|_{L^\infty(L^2)} \\ & \leq A \left(\inf_{\mathbf{v}_h \in V^k} \|\mathbf{u} - \mathbf{v}_h\|_{L^\infty(H(\text{div}))} + \inf_{g_h \in S_p^k} \|p - g_h\|_{L^\infty(L^2)} \right) \\ & \leq A_2 h_p^{k+1} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))} + \|p\|_{L^\infty(H^{k+1})}). \end{aligned}$$

Here A_2 is independent of h_p , u , p , and c .

We let \mathbf{I} be an interpolation operator from $H(\text{div}) \times L_0^2$ to $V^k \times S_p^k$ for $t \in [0, T]$. We use the estimates (4.4) and (4.9) to conclude that

$$(4.10) \quad \begin{aligned} \|\Pi\mathbf{u}\|_{L^\infty(L^\infty)} & \leq \|\Pi\mathbf{u} - \mathbf{I}\mathbf{u}\|_{L^\infty(L^\infty)} + \|\mathbf{I}\mathbf{u} - \mathbf{u}\|_{L^\infty(L^\infty)} + \|\mathbf{u}\|_{L^\infty(L^\infty)} \\ & \leq K_2 h_p^{-1} \|\Pi\mathbf{u} - \mathbf{I}\mathbf{u}\|_{L^\infty(L^2)} + (A_2 + 1) \|\mathbf{u}\|_{L^\infty(L^\infty)} \\ & \leq K_2 h_p^{-1} (\|\Pi\mathbf{u} - \mathbf{u}\|_{L^\infty(L^2)} + \|\mathbf{I}\mathbf{u} - \mathbf{u}\|_{L^\infty(L^2)}) \\ & \quad + (A_2 + 1) \|\mathbf{u}\|_{L^\infty(L^\infty)} \\ & \leq 2A_2 K_2 (\|\mathbf{u}\|_{L^\infty(H^1(\text{div}))} + \|p\|_{L^\infty(H^1)}) \\ & \quad + (A_2 + 1) \|\mathbf{u}\|_{L^\infty(L^\infty)} =: K_4. \end{aligned}$$

For the analysis in section 5 we introduce an extrapolation of the exact velocity \mathbf{u}

$$(4.11) \quad \mathbf{u}^E(\mathbf{x}, t_n^c) := \begin{cases} \left(1 + \frac{t_n^c - t_{m-1}^p}{\Delta t_{m-1}^p}\right) \mathbf{u}(\mathbf{x}, t_{m-1}^p) - \frac{t_n^c - t_{m-1}^p}{\Delta t_{m-1}^p} \mathbf{u}(\mathbf{x}, t_{m-2}^p), \\ N_{m-1} + 1 \leq n \leq N_m, \quad 2 \leq m \leq M, \\ \mathbf{u}(\mathbf{x}, 0), \quad 1 \leq n \leq N_1, \quad m = 1. \end{cases}$$

Then we routinely see that for $2 \leq q \leq +\infty$

$$(4.12) \quad \begin{aligned} & \|\mathbf{u}^E(\mathbf{x}, t) - \mathbf{u}(\mathbf{x}, t)\|_{L^q} \\ & \leq \begin{cases} A_3 (\Delta t_p)^{\frac{3}{2}} \|\mathbf{u}\|_{H^2(t_{m-2}^p, t_m^p; L^q)} & \forall t \in [t_{m-1}^p, t_m^p], \quad m \geq 2, \\ A_3 \Delta t_p^1 \|\mathbf{u}\|_{W_1^\infty(t_0^p, t_1^p; L^q)} & \forall t \in [t_0^p, t_1^p], \quad m = 1. \end{cases} \end{aligned}$$

5. An optimal-order error estimate. In this section we prove an optimal-order error estimate for the ELLAM-MFEM time-stepping procedure with any order of approximating polynomials ($k \geq 0, l \geq 1$).

5.1. On the main theorem and its proof. Note that the test functions in the ELLAM formulation are defined by (3.3), which can be evaluated by using (3.19). However, the velocity \mathbf{u} is unknown. This is in contrast to the ELLAM schemes for

linear transport PDEs in which the true velocity is known and is used to evaluate characteristics [6, 21, 26]. In the ELLAM-MFEM time-stepping procedure in section 3, we have to use the numerical velocity \mathbf{u}_h^E to evaluate the approximate characteristics \mathbf{r}_h by solving problem (3.17). These issues further complicate the analysis [21, 25].

THEOREM 5.1. *Suppose that the solution (c, p, \mathbf{u}) of problem (2.1)–(2.3) satisfies $c \in L^\infty(W_{2+\gamma}^{l+1}) \cap L^\infty(W_\infty^1) \cap H^1(H^{l+1})$ for some $\gamma > 0$, $p \in L^\infty(H^{k+1})$, and $\mathbf{u} \in L^\infty(H^{k+1}(\text{div}) \cap W_\infty^1) \cap W_\infty^1(L^\infty) \cap H^2(L^2)$. Let $(c_h(\mathbf{x}, t_n^c), p_h(\mathbf{x}, t_m^p), \mathbf{u}_h(\mathbf{x}, t_m^p))$ be the solution of the ELLAM-MFEM time-stepping procedure (3.12) and (3.14) with $l \geq 1$ and $k \geq 0$. Assume that the discretization parameters obey the relations*

$$(5.1) \quad \Delta t_c = O(h_p), \quad h_c^{l+1} = o(h_p), \quad \Delta t_p^1 = O(h_p^{2/3}), \quad \Delta t_p = O(h_p^{1/2}).$$

There exist positive constants h_c^ , h_p^* , Δt_c^* , Δt_p^* , and Q^* such that the following optimal-order error estimate holds for $0 < h_c \leq h_c^*$, $0 < h_p \leq h_p^*$, $0 < \Delta t_c \leq \Delta t_c^*$, and $0 < \Delta t_p \leq \Delta t_p^*$:*

$$(5.2) \quad \begin{aligned} & \|c_h - c\|_{\hat{L}_c^\infty(L^2)} + |\mathbf{D}|_{min}^{1/2} \|c_h - c\|_{\hat{L}_c^2(H^1)} \\ & \quad + \|\mathbf{u}_h - \mathbf{u}\|_{\hat{L}_p^\infty(H(\text{div}))} + \|p_h - p\|_{\hat{L}_p^\infty(L^2)} \\ & \leq Q^* \Delta t_c \left(\|\bar{c}\|_{L^2(L^2)} + \|c\|_{L^2(H^1)} + \left\| \frac{d\bar{c}}{dt} \right\|_{L^2(L^2)} + \left\| \frac{dc}{dt} \right\|_{L^2(H^1)} \right) \\ & \quad + Q^* ((\Delta t_p^1)^{3/2} + (\Delta t_p)^2) \|\mathbf{u}\|_{H^2(L^2)} + Q^* h_c^{l+1} (\|c\|_{L^\infty(W_{2+\gamma}^{l+1})} \\ & \quad + \|c\|_{H^1(H^{l+1})}) + Q^* h_p^{k+1} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))} + \|p\|_{L^\infty(H^{k+1})}). \end{aligned}$$

Here $\frac{d}{dt}$ refers to the material derivative along the characteristics defined in (3.4). The constant $Q^* = Q^*(h_c^*, h_p^*, \Delta t_c^*, \Delta t_p^*, T)$, but Q^* is independent of the discretization parameters h_c , h_p , Δt_c , or Δt_p .

To prove the theorem, we use (3.10), (3.12), and (4.8) to derive a relation

$$\begin{aligned} & \int_\Omega \mu(c_h(\mathbf{x}, t_m^p)) \mathbf{K}^{-1}(\mathbf{x}) (\mathbf{u}_h(\mathbf{x}, t_m^p) - \Pi \mathbf{u}(\mathbf{x}, t_m^p)) \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x} \\ & \quad - \int_\Omega (p_h(\mathbf{x}, t_m^p) - \Pi p(\mathbf{x}, t_m^p)) \nabla \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x} \\ & = \int_\Omega (\mu(c(\mathbf{x}, t_m^p)) - \mu(c_h(\mathbf{x}, t_m^p))) \mathbf{K}^{-1}(\mathbf{x}) \Pi \mathbf{u}(\mathbf{x}, t_m^p) \cdot \mathbf{v}_h(\mathbf{x}) d\mathbf{x}, \\ & \int_\Omega w_h(\mathbf{x}) \nabla \cdot (\mathbf{u}_h(\mathbf{x}, t_m^p) - \Pi \mathbf{u}(\mathbf{x}, t_m^p)) d\mathbf{x} = 0 \quad \forall (\mathbf{v}_h, w_h) \in V^k \times S_p^k. \end{aligned}$$

Combining this equation with (4.10) yields an estimate [4, 5, 8]

$$(5.3) \quad \begin{aligned} & \|\mathbf{u}_h(\mathbf{x}, t_m^p) - \Pi \mathbf{u}(\mathbf{x}, t_m^p)\|_{H(\text{div})} + \|p_h(\mathbf{x}, t_m^p) - \Pi p(\mathbf{x}, t_m^p)\| \\ & \leq Q(1 + \|\Pi \mathbf{u}(\mathbf{x}, t_m^p)\|_{L^\infty}) \|c_h(\mathbf{x}, t_m^p) - c(\mathbf{x}, t_m^p)\| \\ & \leq Q_1 \|c_h(\mathbf{x}, t_m^p) - c(\mathbf{x}, t_m^p)\|, \quad 0 \leq m \leq M. \end{aligned}$$

For convenience, we have dropped the subscript L^2 .

The estimates (4.9) and (5.3) show that the bound on $\|\mathbf{u}_h - \mathbf{u}\|_{\dot{L}^\infty_p(H(\text{div}))} + \|p_h - p\|_{\dot{L}^\infty_p(L^2)}$ in (5.2) is a consequence of the bound on $\|c_h - c\|_{\dot{L}^\infty(L^2)}$.

5.2. Proof of the key estimate. To bound $\|c_h - c\|_{\dot{L}^\infty(L^2)}$, we set $\xi(\mathbf{x}, t_n^c) := c_h(\mathbf{x}, t_n^c) - \Pi c(\mathbf{x}, t_n^c)$ and $\eta(\mathbf{x}, t_n^c) := \Pi c(\mathbf{x}, t_n^c) - c(\mathbf{x}, t_n^c)$. Note that $c_h - c = \xi + \eta$ and that the estimate for η is known from (4.6). The key to prove the theorem is to derive an estimate of the form (5.2) for ξ .

Proof. We subtract (3.14) from (3.9) for $n = N_{m-1} + 1, \dots, N_m$ to generate an error equation for any $z_h(\mathbf{x}, t_n^c) \in S_c^l$

$$\begin{aligned} & \int_{\Omega} \phi(\mathbf{x})(c_h(\mathbf{x}, t_n^c) - c(\mathbf{x}, t_n^c))z_h(\mathbf{x}, t_n^c) d\mathbf{x} \\ & + \Delta t_n^c \int_{\Omega} \nabla z_h(\mathbf{x}, t_n^c) \cdot (\mathbf{D}(\mathbf{x}, \mathbf{u}_h^E(\mathbf{x}, t_n^c)) \nabla c_h(\mathbf{x}, t_n^c) - \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c)) \nabla c(\mathbf{x}, t_n^c)) d\mathbf{x} \\ = & \int_{\Omega} \phi(\mathbf{x})(c_h(\mathbf{x}, t_{n-1}^c) - c(\mathbf{x}, t_{n-1}^c))z_h(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} \\ & + \Delta t_n^c \int_{\Omega} (\bar{c}_h(\mathbf{x}, t_n^c) - \bar{c}(\mathbf{x}, t_n^c))q(\mathbf{x}, t_n^c)z_h(\mathbf{x}, t_n^c) d\mathbf{x} \\ & + E_{\mathbf{D}}(c, z_h) - E_q(\bar{c}, z_h). \end{aligned}$$

In the second term on the right-hand side, $\bar{c}_h := \bar{c}$ is specified at sources so the difference $\bar{c}_h - \bar{c}$ vanishes. At sinks $q = q^-$ is specified but $\bar{c}_h = c_h$ and $\bar{c} = c$. We rewrite the preceding equation with $z_h = \xi$ as

$$\begin{aligned} & \int_{\Omega} \phi(\mathbf{x})\xi^2(\mathbf{x}, t_n^c) d\mathbf{x} + \Delta t_n^c \int_{\Omega} \nabla \xi(\mathbf{x}, t_n^c) \cdot \mathbf{D}(\mathbf{x}, \mathbf{u}_h^E(\mathbf{x}, t_n^c)) \nabla \xi(\mathbf{x}, t_n^c) d\mathbf{x} \\ = & \int_{\Omega} \phi(\mathbf{x})\xi(\mathbf{x}, t_{n-1}^c)\xi(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} + \int_{\Omega} \phi(\mathbf{x})\eta(\mathbf{x}, t_{n-1}^c)\xi(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} \\ (5.4) \quad & + \Delta t_n^c \int_{\Omega} q^-(\mathbf{x}, t_n^c)\xi^2(\mathbf{x}, t_n^c) d\mathbf{x} + \Delta t_n^c \int_{\Omega} q^-(\mathbf{x}, t_n^c)\eta(\mathbf{x}, t_n^c)\xi(\mathbf{x}, t_n^c) d\mathbf{x} \\ & - \Delta t_n^c \int_{\Omega} \nabla \xi(\mathbf{x}, t_n^c) \cdot (\mathbf{D}(\mathbf{x}, \mathbf{u}_h^E(\mathbf{x}, t_n^c)) - \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c))) \nabla \Pi c(\mathbf{x}, t_n^c) d\mathbf{x} \\ & - \Delta t_n^c \int_{\Omega} \nabla \xi(\mathbf{x}, t_n^c) \cdot \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c)) \nabla \eta(\mathbf{x}, t_n^c) d\mathbf{x} \\ & - \int_{\Omega} \phi(\mathbf{x})\eta(\mathbf{x}, t_n^c)\xi(\mathbf{x}, t_n^c) d\mathbf{x} + E_{\mathbf{D}}(c, \xi) - E_q(\bar{c}, \xi). \end{aligned}$$

We bound the third and fourth terms on the right-hand side of (5.4) by

$$\begin{aligned} & \left| \Delta t_n^c \int_{\Omega} q^-(\mathbf{x}, t_n^c)\xi^2(\mathbf{x}, t_n^c) d\mathbf{x} + \Delta t_n^c \int_{\Omega} q^-(\mathbf{x}, t_n^c)\eta(\mathbf{x}, t_n^c)\xi(\mathbf{x}, t_n^c) d\mathbf{x} \right| \\ & \leq Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 + \Delta t_n^c \|\eta(\mathbf{x}, t_n^c)\|^2 \\ & \leq Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 + A_1^2 \Delta t_n^c h_c^{2l+2} \|c\|_{L^\infty(H^{l+1})}^2. \end{aligned}$$

We use (4.5) and (4.6) to bound the sixth term on the right-hand side of (5.4)

$$\begin{aligned} & \left| \Delta t_n^c \int_{\Omega} \nabla \xi(\mathbf{x}, t_n^c) \cdot \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c)) \nabla \eta(\mathbf{x}, t_n^c) d\mathbf{x} \right| \\ &= \left| \Delta t_n^c \int_{\Omega} \xi(\mathbf{x}, t_n^c) \eta(\mathbf{x}, t_n^c) d\mathbf{x} \right| \\ &\leq Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 + \Delta t_n^c \|\eta(\mathbf{x}, t_n^c)\|^2 \\ &\leq Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 + A_1^2 \Delta t_n^c h_c^{2l+2} \|c\|_{L^\infty(H^{l+1})}^2. \end{aligned}$$

The fifth term on the right-hand side of (5.4) is bounded in Lemma 6.3

$$\begin{aligned} & \left| \Delta t_n^c \int_{\Omega} \nabla \xi(\mathbf{x}, t_n^c) \cdot (\mathbf{D}(\mathbf{x}, \mathbf{u}_h^E(\mathbf{x}, t_n^c)) - \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c))) \nabla \Pi c(\mathbf{x}, t_n^c) d\mathbf{x} \right| \\ (5.5) \quad & \leq \varepsilon \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 + Q \Delta t_n^c (\|\xi(\mathbf{x}, t_{m-1}^p)\|^2 + \|\xi(\mathbf{x}, t_{m-2}^p)\|^2) \\ & \quad + Q \Delta t_n^c \left(h_c^{2l+2} \|c\|_{L^\infty(H^{l+1})}^2 + h_p^{2k+2} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))}^2 + \|p\|_{L^\infty(H^{k+1})}^2) \right) \\ & \quad + \delta_{m,1} (\Delta t_p^1)^2 \|\mathbf{u}\|_{W_1^\infty(0, t_p^1; L^2)}^2 + (1 - \delta_{m,1}) (\Delta t_p)^3 \|\mathbf{u}\|_{H^2(t_{m-2}^p, t_m^p; L^2)}^2, \end{aligned}$$

where $\delta_{i,j} = 1$ if $i = j$ or 0 otherwise.

Note that the evaluation of source and sink terms and the diffusion-dispersion term in the ELLAM scheme (3.14) does not involve any characteristic tracking. Hence, (3.6) and (3.8) still hold, leading to the estimate

$$\begin{aligned} |E_q(\bar{c}, \xi)| &= \left| \int_{\Omega} \xi(\mathbf{x}, t_n^c) \int_{t_{n-1}^c}^{t_n^c} \left\{ \int_{\theta}^{t_n^c} \frac{d}{dt} (\bar{c}(\mathbf{r}(t; \mathbf{x}, t_n^c), t) q(\mathbf{r}(t; \mathbf{x}, t_n^c), t)) dt \right. \right. \\ & \quad \left. \left. + \bar{c}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) q(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta) \left[\det \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right) - 1 \right] \right\} d\theta d\mathbf{x} \right| \\ &\leq Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 + Q (\Delta t_n^c)^2 \left(\|\bar{c}\|_{L^2(t_{n-1}^c, t_n^c; L^2)}^2 + \left\| \frac{d\bar{c}}{dt} \right\|_{L^2(t_{n-1}^c, t_n^c; L^2)}^2 \right). \end{aligned}$$

We use the estimates (6.1) and (6.2) in Lemma 6.1 to bound $|E_D(c, \xi)|$ by

$$\begin{aligned} |E_D(c, \xi)| &\leq \left| \int_{\Omega} \int_{t_{n-1}^c}^{t_n^c} \left(\det \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right) \left(\frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_n^c)}{\partial \mathbf{x}} \right)^{-1} - \mathbf{I} \right) \nabla \xi(\mathbf{x}, t_n^c) \right. \\ & \quad \left. \cdot (\mathbf{D}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta)) \nabla c(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta)) d\theta d\mathbf{x} \right| \\ & \quad + \left| \int_{\Omega} \int_{t_{n-1}^c}^{t_n^c} \nabla \xi(\mathbf{x}, t_n) \cdot (\mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c)) \nabla c(\mathbf{x}, t_n^c) \right. \\ & \quad \left. - \mathbf{D}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta)) \nabla c(\mathbf{r}(\theta; \mathbf{x}, t_n^c), \theta)) d\theta d\mathbf{x} \right| \\ &\leq \varepsilon \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 + Q (\Delta t_n^c)^2 \left(\|c\|_{L^2(t_{n-1}^c, t_n^c; H^1)}^2 + \left\| \frac{dc}{dt} \right\|_{L^2(t_{n-1}^c, t_n^c; H^1)}^2 \right). \end{aligned}$$

The first term on the right-hand side of (5.4) is estimated in Lemma 6.4

$$\begin{aligned}
 & \left| \int_{\Omega} \phi(\mathbf{x}) \xi(\mathbf{x}, t_{n-1}^c) \xi(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} \right| \\
 (5.6) \quad & \leq \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_{n-1}^c) d\mathbf{x} + \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_n^c) d\mathbf{x} + \varepsilon \Delta t_n^c (\|\nabla \xi(\mathbf{x}, t_n^c)\|^2 \\
 & \quad + \|\nabla \xi(\mathbf{x}, t_{n-1}^c)\|^2) + Q \Delta t_n^c (\|\xi(\mathbf{x}, t_n^c)\|^2 + \|\xi(\mathbf{x}, t_{n-1}^c)\|^2).
 \end{aligned}$$

The second and seventh terms on the right-hand side of (5.4) are estimated in Lemma 6.5

$$\begin{aligned}
 & \left| \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_n^c) \xi(\mathbf{x}, t_n^c) d\mathbf{x} - \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_{n-1}^c) \xi(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} \right| \\
 (5.7) \quad & \leq \varepsilon \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 + Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 \\
 & \quad + Q h_c^{2l+2} \|c\|_{H^1(t_{n-1}^c, t_n^c; H^{l+1})}^2 + Q \Delta t_n^c h_c^{2l+2} \|c\|_{L^\infty(W_{2+\gamma}^{l+1})}^2.
 \end{aligned}$$

We incorporate the preceding estimates into (5.4) to get

$$\begin{aligned}
 & \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_n^c) d\mathbf{x} + |\mathbf{D}|_{min} \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 \\
 & \leq \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_n^c) d\mathbf{x} + \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_{n-1}^c) d\mathbf{x} + 3\varepsilon \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 \\
 & \quad + \varepsilon \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_{n-1}^c)\|^2 + Q \Delta t_n^c (\|\xi(\mathbf{x}, t_n^c)\|^2 + \|\xi(\mathbf{x}, t_{n-1}^c)\|^2 \\
 (5.8) \quad & \quad + \|\xi(\mathbf{x}, t_{m-1}^p)\|^2 + \|\xi(\mathbf{x}, t_{m-2}^p)\|^2) + Q (\Delta t_n^c)^2 (\|\bar{c}\|_{L^2(t_{n-1}^c, t_n^c; L^2)}^2 \\
 & \quad + \|c\|_{L^2(t_{n-1}^c, t_n^c; H^1)}^2 + \left\| \frac{d\bar{c}}{dt} \right\|_{L^2(t_{n-1}^c, t_n^c; L^2)}^2 + \left\| \frac{dc}{dt} \right\|_{L^2(t_{n-1}^c, t_n^c; H^1)}^2) \\
 & \quad + Q \Delta t_n^c (\delta_{m,1} (\Delta t_p^1)^2 \|\mathbf{u}\|_{W_\infty^1(0, t_p^1; L^2)}^2 + (1 - \delta_{m,1}) (\Delta t_p)^3 \|\mathbf{u}\|_{H^2(t_{m-2}^p, t_m^p; L^2)}^2) \\
 & \quad + Q h_c^{2l+2} (\Delta t_n^c \|c\|_{L^\infty(W_{2+\gamma}^{l+1})}^2 + \|c\|_{H^1(t_{n-1}^c, t_n^c; H^{l+1})}^2) \\
 & \quad + Q \Delta t_n^c h_p^{2k+2} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))}^2 + \|p\|_{L^\infty(H^{k+1})}^2).
 \end{aligned}$$

We choose $\varepsilon = |\mathbf{D}|_{min}/8$, sum this estimate for $n = 1, 2, \dots, n^*$, with $n^* \leq N_m$, and cancel like terms to obtain

$$\begin{aligned}
 & \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_{n^*}^c) d\mathbf{x} + |\mathbf{D}|_{min} \sum_{n=1}^{n^*} \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 \\
 (5.9) \quad & \leq Q \sum_{n=1}^{n^*} \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 + Q (\Delta t_n^c)^2 (\|\bar{c}\|_{L^2(L^2)}^2 + \|c\|_{L^2(H^1)}^2 \\
 & \quad + \left\| \frac{d\bar{c}}{dt} \right\|_{L^2(L^2)}^2 + \left\| \frac{dc}{dt} \right\|_{L^2(H^1)}^2) + Q ((\Delta t_p)^4 + (\Delta t_p^1)^3) \|\mathbf{u}\|_{H^2(L^2)}^2 \\
 & \quad + Q h_c^{2l+2} (\|c\|_{L^\infty(W_{2+\gamma}^{l+1})}^2 + \|c\|_{H^1(H^{l+1})}^2) \\
 & \quad + Q h_p^{2k+2} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))}^2 + \|p\|_{L^\infty(H^{k+1})}^2).
 \end{aligned}$$

Here we have used the estimate (6.8) to bound the initial value $\|\xi(\mathbf{x}, 0)\|$ that has appeared on the right-hand side.

We choose Δt_n^c small enough such that $Q\Delta t_n^c < \phi_{\min}/2$ and apply Gronwall inequality to (5.9) to get

$$\begin{aligned}
 & \|\xi\|_{\hat{L}^\infty(0, t_{n^*}^c; L^2)}^2 + |\mathbf{D}|_{\min} \|\nabla \xi\|_{\hat{L}^2(0, t_{n^*}^c; L^2)}^2 \\
 (5.10) \quad & \leq Q(\Delta t_n^c)^2 \left(\|\bar{c}\|_{L^2(L^2)}^2 + \|c\|_{L^2(H^1)}^2 + \left\| \frac{d\bar{c}}{dt} \right\|_{L^2(L^2)}^2 + \left\| \frac{dc}{dt} \right\|_{L^2(H^1)}^2 \right) \\
 & \quad + Q((\Delta t_p)^4 + (\Delta t_p^1)^3) \|\mathbf{u}\|_{H^2(L^2)}^2 + Qh_c^{2l+2} (\|c\|_{L^\infty(W_{2+\gamma}^{l+1})}^2 + \|c\|_{H^1(H^{l+1})}^2) \\
 & \quad + Qh_p^{2k+2} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))}^2 + \|p\|_{L^\infty(H^{k+1})}^2).
 \end{aligned}$$

Combining this estimate with (4.6) finishes the proof. \square

5.3. Discussion. The error estimate (5.2) contains only the H^1 norm of c and its material derivative in the Δt_c term. These norms are much smaller than those of the temporal derivatives c due to the Lagrangian nature of the transport PDEs. Hence, larger time steps and spatial grids can be used in the ELLAM-MFEM time-stepping procedure. In other words, Theorem 5.1 theoretically justifies the mathematical and numerical strength of the ELLAM-MFEM time-stepping procedure, which was previously observed numerically [3, 17, 21, 30, 32].

In the ELLAM-MFEM time-stepping procedure (3.12) and (3.14), a linear extrapolation in time is used to define the numerical velocity field $\mathbf{u}_h^E(\mathbf{x}, t_n^c)$ in (3.13). A constant-in-time interpolation can be used instead:

$$\mathbf{u}_h^E(\mathbf{x}, t_n^c) := \mathbf{u}_h(\mathbf{x}, t_{m-1}^p) \quad \text{for } N_{m-1} + 1 \leq n \leq N_m, \quad 1 \leq m \leq M.$$

The proof in Theorem 5.1 still goes through, leading to an estimate of the form

$$\begin{aligned}
 & \|c_h - c\|_{\hat{L}^\infty(L^2)} + \|\mathbf{u}_h - \mathbf{u}\|_{\hat{L}_p^\infty(H(\text{div}))} + \|p_h - p\|_{\hat{L}_p^\infty(L^2)} \\
 & \leq Q(h_c^{l+1} + h_p^{k+1} + \Delta t_c + \Delta t_p).
 \end{aligned}$$

An error estimate similar to Theorem 5.1 was proved in [9] for a Galerkin FEM-MFEM time-stepping procedure for problem (2.1)–(2.3) and in [13] for an MMOC-MFEM time-stepping procedure. These estimates require a restrictive condition that

$$(5.11) \quad \Delta t_c = o(h_p).$$

In other words, these procedures are guaranteed to converge only if the Courant number tends to zero asymptotically, which is more restrictive than the CFL condition for an explicit scheme. This is especially important for the MMOC-MFEM time-stepping procedure, since the strength of the MMOC scheme is really reflected in the large time steps the MMOC scheme allows.

In Theorem 5.1 the restriction (5.11) is relaxed to be

$$(5.12) \quad \Delta t_c = O(h_p).$$

This implies that the ELLAM-MFEM time-stepping procedure converges for any size of Courant numbers. Thus, Theorem 5.1 provides a solid theoretical foundation to show the competitiveness of the ELLAM-MFEM procedure, which was previously illustrated and observed numerically [21, 30, 32].

6. Auxiliary lemmas. In this section we prove several lemmas that were used in the proof of Theorem 5.1.

6.1. Estimates on tracking. In this subsection, we derive various bounds for tracking-related transformations.

LEMMA 6.1. Assume that $\phi \in W_\infty^1$ and $\mathbf{u} \in L^\infty(W_\infty^1)$. Then the Jacobian matrix of the characteristic $\mathbf{r}(t; \mathbf{x}, t_{n-1}^c)$ is bounded in the Frobenius norm $|\cdot|_2$ by

$$(6.1) \quad \left| \frac{\partial \mathbf{r}(t; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} - \mathbf{I} \right|_2 \leq Q(t - t_{n-1}^c), \quad t \in [t_{n-1}^c, t_n^c].$$

Here Q depends on $\|\mathbf{u}\|_{L^\infty(W_\infty^1)}$ but not on discretization parameters. In addition,

$$(6.2) \quad \det \left(\frac{\partial \mathbf{r}(t; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} \right) = 1 + O(t - t_{n-1}^c), \quad t \in [t_{n-1}^c, t_n^c].$$

Proof. Differentiating (3.15) with respect to \mathbf{x} yields, for $t \in [t_{n-1}^c, t_n^c]$,

$$(6.3) \quad \frac{\partial \mathbf{r}(t; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} - \mathbf{I} = \int_{t_{n-1}^c}^t \nabla \left(\frac{\mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c), \theta)}{\phi(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c), \theta)} \right) \frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} d\theta.$$

We apply Cauchy inequality to bound the Frobenius norm of $\frac{\partial \mathbf{r}}{\partial \mathbf{x}} - \mathbf{I}$ by

$$\begin{aligned} \left| \frac{\partial \mathbf{r}(t; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} - \mathbf{I} \right|_2^2 &\leq (t - t_{n-1}^c) \int_{t_{n-1}^c}^t \left| \nabla \left(\frac{\mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c), \theta)}{\phi(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c), \theta)} \right) \frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} \right|_2^2 d\theta \\ &\leq (t - t_{n-1}^c) \left\| \frac{\mathbf{u}}{\phi} \right\|_{L^\infty(W_\infty^1)}^2 \int_{t_{n-1}^c}^t \left| \frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} \right|_2^2 d\theta \\ &\leq Q(t - t_{n-1}^c)^2 + Q(t - t_{n-1}^c) \int_{t_{n-1}^c}^t \left| \frac{\partial \mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c)}{\partial \mathbf{x}} - \mathbf{I} \right|_2^2 d\theta. \end{aligned}$$

Applying Gronwall inequality finishes the proof of (6.1), which directly gives (6.2). \square

LEMMA 6.2. Under the assumptions of Theorem 5.1,

$$(6.4) \quad h_p^{-1} h_c^{l+1} \|c_0\|_{H^{l+1}} \leq 1,$$

and

$$(6.5) \quad \frac{\Delta t_c}{h_p} \leq Q_2, \quad \frac{\Delta t_p}{h_p^{1/2}} \leq Q_2, \quad \frac{\Delta t_p^1}{h_p^{2/3}} \leq Q_2,$$

we have the following estimate for the difference $\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}$:

$$(6.6) \quad \|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\|_{L^q} \leq Q_3 \Delta t_n^c h_p^{\frac{2}{q}}.$$

Proof. We use (3.15) and (3.18) and the estimates (4.3) and (5.3) to bound $\|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\|_{L^q}$ for $2 \leq q \leq +\infty$ by

$$\begin{aligned}
\|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\|_{L^q} &= \left\| \frac{\mathbf{u}_h^E(\mathbf{x}, t_{n-1}^c)}{\phi(\mathbf{x})} \Delta t_n^c - \int_{t_{n-1}^c}^{t_n^c} \frac{\mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c), \theta)}{\phi(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c))} d\theta \right\|_{L^q} \\
(6.7) \quad &= \left\| \Delta t_n^c \left(\frac{\mathbf{u}_h^E(\mathbf{x}, t_{n-1}^c) - \mathbf{u}^E(\mathbf{x}, t_{n-1}^c)}{\phi(\mathbf{x})} + \frac{\mathbf{u}^E(\mathbf{x}, t_{n-1}^c) - \mathbf{u}(\mathbf{x}, t_{n-1}^c)}{\phi(\mathbf{x})} \right) \right. \\
&\quad \left. - \int_{t_{n-1}^c}^{t_n^c} \left(\frac{\mathbf{u}(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c), \theta)}{\phi(\mathbf{r}(\theta; \mathbf{x}, t_{n-1}^c))} - \frac{\mathbf{u}(\mathbf{x}, t_{n-1}^c)}{\phi(\mathbf{x})} \right) d\theta \right\|_{L^q} \\
&\leq 3\phi_{\min}^{-1} \Delta t_n^c \left(\|\mathbf{u}_h - \mathbf{u}\|_{\hat{L}_p^\infty(t_{m-2}^p, t_{m-1}^p; L^q)} + \delta_{m,1} \Delta t_p^1 \|\mathbf{u}\|_{W_1^\infty(t_0^p, t_1^p; L^q)} \right. \\
&\quad \left. + (1 - \delta_{m,1})(\Delta t_p)^{3/2} \|\mathbf{u}\|_{H^2(t_{m-2}^p, t_m^p; L^q)} + Q \Delta t_n^c \right).
\end{aligned}$$

Here Q depends on $\|\frac{d\mathbf{u}}{dt}\|_{L^\infty(L^\infty)}$ and $\|\mathbf{u}\|_{L^\infty(L^\infty)}$ but not on discretization parameters.

We combine (4.1), (4.6), and (5.3) to conclude that

$$\begin{aligned}
(6.8) \quad \|\xi(\mathbf{x}, 0)\| &\leq \|c_h(\mathbf{x}, 0) - \Pi c_0(\mathbf{x})\| \\
&\leq \|c_h(\mathbf{x}, 0) - c_0(\mathbf{x})\| + \|\Pi c_0(\mathbf{x}) - c_0(\mathbf{x})\| \leq 2A_1 h_c^{l+1} \|c_0\|_{H^{l+1}}
\end{aligned}$$

and

$$\begin{aligned}
(6.9) \quad &\|(\mathbf{u}_h - \Pi \mathbf{u})(\mathbf{x}, 0)\|_{L^q} \\
&\leq K_2 h_p^{-(1-\frac{2}{q})} \|(\mathbf{u}_h - \Pi \mathbf{u})(\mathbf{x}, 0)\| \leq K_2 Q_1 h_p^{-(1-\frac{2}{q})} \|c_h(\mathbf{x}, 0) - c_0(\mathbf{x})\| \\
&\leq A_1 K_2 Q_1 h_p^{-(1-\frac{2}{q})} h_c^{l+1} \|c_0\|_{H^{l+1}} \leq A_1 K_2 Q_1 h_p^{\frac{2}{q}},
\end{aligned}$$

provided that condition (6.4) is true.

By (4.4) and (5.1), the estimate (6.7) reduces to the following for $n = 1, 2, \dots, N_1$:

$$\begin{aligned}
(6.10) \quad \|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\|_{L^q} &\leq 3\phi_{\min}^{-1} \Delta t_n^c \left(\|(\mathbf{u}_h - \mathbf{u})(\mathbf{x}, 0)\|_{L^q} + \Delta t_p^1 \|\mathbf{u}\|_{W_1^\infty(t_0^p, t_1^p; L^q)} + Q \Delta t_n^c \right) \\
&\leq 3\phi_{\min}^{-1} \Delta t_n^c \left(A_2 K_2 h_p^{k+\frac{2}{q}} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))} + \|p\|_{L^\infty(H^{k+1})}) \right. \\
&\quad \left. + A_1 K_2 Q_1 h_p^{\frac{2}{q}} + \Delta t_p^1 \|\mathbf{u}\|_{W_1^\infty(t_0^p, t_1^p; L^q)} + Q \Delta t_n^c \right) \\
&\leq Q_4 \Delta t_n^c h_p^{\frac{2}{q}}.
\end{aligned}$$

For $n = N_{m-1} + 1, 2, \dots, N_m$, we use (4.4), (5.1), (5.2), and (6.5) to bound (6.7) as follows:

$$\begin{aligned}
(6.11) \quad &\|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\|_{L^q} \\
&\leq 3\phi_{\min}^{-1} \Delta t_n^c \left[\|\mathbf{u}_h - \mathbf{u}\|_{\hat{L}_p^\infty(t_{m-2}^p, t_{m-1}^p; L^q)} + \delta_{m,1} \Delta t_p^1 \|\mathbf{u}\|_{W_1^\infty(t_0^p, t_1^p; L^q)} \right. \\
&\quad \left. + (1 - \delta_{m,1})(\Delta t_p)^{3/2} \|\mathbf{u}\|_{H^2(t_{m-2}^p, t_m^p; L^q)} + Q \Delta t_n^c \right] \\
&\leq 3\phi_{\min}^{-1} \Delta t_n^c h_p^{\frac{2}{q}} \left[(A_2 + Q^*) K_2 h_p^k (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))} + \|p\|_{L^\infty(H^{k+1})}) \right. \\
&\quad \left. + Q^* Q_2 \left(\|\bar{c}\|_{L^2(L^2)} + \|c\|_{L^2(H^1)} + \left\| \frac{d\bar{c}}{d\tau} \right\|_{L^2(L^2)} + \left\| \frac{dc}{d\tau} \right\|_{L^2(H^1)} \right) \right. \\
&\quad \left. + Q^* Q_2 \|\mathbf{u}\|_{H^2(L^2)} + Q^* \right] \\
&\leq Q_3 \Delta t_n^c h_p^{\frac{2}{q}}. \quad \square
\end{aligned}$$

6.2. Miscellaneous estimates. In this subsection we prove the estimates (5.5), (5.6), and (5.7) for the fifth, the first, and the second and seventh terms on the right-hand side of (5.4), respectively.

LEMMA 6.3. *Under the conditions of Theorem 5.1, estimate (5.5) holds for $n = N_{m-1} + 1, \dots, N_m$.*

Proof. It is straightforward to see that [8]

$$|\mathbf{D}(\mathbf{x}, \mathbf{u}) - \mathbf{D}(\mathbf{x}, \mathbf{v})| \leq Q_4 |\mathbf{u} - \mathbf{v}|.$$

With this we bound the left-hand side of (5.5) by

$$\begin{aligned} & \left| \Delta t_n^c \int_{\Omega} \nabla \xi(\mathbf{x}, t_n^c) \cdot (\mathbf{D}(\mathbf{x}, \mathbf{u}_h^E(\mathbf{x}, t_n^c)) - \mathbf{D}(\mathbf{x}, \mathbf{u}(\mathbf{x}, t_n^c))) \nabla \Pi c(\mathbf{x}, t_n^c) d\mathbf{x} \right| \\ (6.12) \quad & \leq Q_4 \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\| \|\mathbf{u}_h^E(\mathbf{x}, t_n^c) - \mathbf{u}(\mathbf{x}, t_n^c)\| \|\Pi c(\mathbf{x}, t_n^c)\|_{W_{\infty}^1} \\ & \leq K_3 Q_4 \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\| (\|\mathbf{u}_h^E(\mathbf{x}, t_n^c) - (\Pi \mathbf{u})^E(\mathbf{x}, t_n^c)\| \\ & \quad + \|(\Pi \mathbf{u})^E(\mathbf{x}, t_n^c) - \mathbf{u}^E(\mathbf{x}, t_n^c)\| + \|\mathbf{u}^E(\mathbf{x}, t_n^c) - \mathbf{u}(\mathbf{x}, t_n^c)\|), \end{aligned}$$

where at the last “ \leq ” sign we have used (4.7).

The last term in the bracket is bounded in (4.12). We use the estimate (4.9) to bound the second term in the bracket to get

$$\begin{aligned} & \|(\Pi \mathbf{u})^E(\mathbf{x}, t_n^c) - \mathbf{u}^E(\mathbf{x}, t_n^c)\| \\ & \leq Q (\|\Pi \mathbf{u}(\mathbf{x}, t_{m-2}^p) - \mathbf{u}(\mathbf{x}, t_{m-2}^p)\| + \|\Pi \mathbf{u}(\mathbf{x}, t_{m-1}^p) - \mathbf{u}(\mathbf{x}, t_{m-1}^p)\|) \\ & \leq Q h_p^{k+1} (\|\mathbf{u}\|_{L^\infty(H^{k+1}(\text{div}))} + \|p\|_{L^\infty(H^{k+1})}). \end{aligned}$$

We use (4.6) and (5.3) to bound the first term in the bracket of (6.12) by

$$\begin{aligned} & \|\mathbf{u}_h^E(\mathbf{x}, t_n^c) - (\Pi \mathbf{u})^E(\mathbf{x}, t_n^c)\| \\ & \leq Q (\|\mathbf{u}_h(\mathbf{x}, t_{m-2}^p) - \Pi \mathbf{u}(\mathbf{x}, t_{m-2}^p)\| + \|\mathbf{u}_h(\mathbf{x}, t_{m-1}^p) - \Pi \mathbf{u}(\mathbf{x}, t_{m-1}^p)\|) \\ & \leq Q (\|c_h(\mathbf{x}, t_{m-2}^p) - c(\mathbf{x}, t_{m-2}^p)\| + \|c_h(\mathbf{x}, t_{m-1}^p) - c(\mathbf{x}, t_{m-1}^p)\|) \\ & \leq Q (\|\xi(\mathbf{x}, t_{m-2}^p)\| + \|\xi(\mathbf{x}, t_{m-1}^p)\|) + Q h_c^{l+1} \|c\|_{L^\infty(H^{l+1})}. \end{aligned}$$

We combine these two estimates with (4.12) to complete the proof. \square

LEMMA 6.4. *Under the conditions of Theorem 5.1, estimate (5.6) holds for $n = N_{m-1} + 1, \dots, N_m$.*

Proof. The first term on the right-hand side of (5.4) can be written as

$$\begin{aligned} & \int_{\Omega} \phi(\mathbf{x}) \xi(\mathbf{x}, t_{n-1}^c) \xi(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} = \int_{\Omega} \phi(\mathbf{x}) \xi(\mathbf{x}, t_{n-1}^c) \xi(\tilde{\mathbf{x}}_h, t_n^c) d\mathbf{x} \\ (6.13) \quad & = \int_{\Omega} \phi(\mathbf{x}) \xi(\mathbf{x}, t_{n-1}^c) \xi(\tilde{\mathbf{x}}, t_n^c) d\mathbf{x} \\ & \quad + \int_{\Omega} \phi(\mathbf{x}) \xi(\mathbf{x}, t_{n-1}^c) (\xi(\tilde{\mathbf{x}}_h, t_n^c) - \xi(\tilde{\mathbf{x}}, t_n^c)) d\mathbf{x}. \end{aligned}$$

We use estimate (6.2) to bound the first term on the right-hand side of (6.13)

$$\begin{aligned}
 & \left| \int_{\Omega} \phi(\mathbf{x}) \xi(\mathbf{x}, t_{n-1}^c) \xi(\tilde{\mathbf{x}}, t_n^c) d\mathbf{x} \right| \\
 & \leq \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_{n-1}^c) d\mathbf{x} + \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\tilde{\mathbf{x}}, t_n^c) d\mathbf{x} \\
 (6.14) \quad & = \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_{n-1}^c) d\mathbf{x} + \frac{1}{2} \int_{\Omega} \phi(\tilde{\mathbf{x}}) \xi^2(\tilde{\mathbf{x}}, t_n^c) \det\left(\frac{\partial \mathbf{x}}{\partial \tilde{\mathbf{x}}}\right) d\tilde{\mathbf{x}} \\
 & \quad + \frac{1}{2} \int_{\Omega} (\phi(\mathbf{x}) - \phi(\tilde{\mathbf{x}})) \xi^2(\tilde{\mathbf{x}}, t_n^c) \det\left(\frac{\partial \mathbf{x}}{\partial \tilde{\mathbf{x}}}\right) d\tilde{\mathbf{x}} \\
 & \leq \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_{n-1}^c) d\mathbf{x} + \frac{1}{2} \int_{\Omega} \phi(\mathbf{x}) \xi^2(\mathbf{x}, t_n^c) d\mathbf{x} + Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2.
 \end{aligned}$$

Here we have rewritten $\tilde{\mathbf{x}}$ as \mathbf{x} in the second term.

We use (4.2), (6.6), and the relationship

$$(6.15) \quad \xi(\tilde{\mathbf{x}}_h, t_n^c) - \xi(\tilde{\mathbf{x}}, t_n^c) = (\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}) \cdot \int_0^1 \nabla \xi(\tilde{\mathbf{x}} + s(\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}), t_n^c) ds,$$

to bound the second term on the right-hand side of (6.13) by

$$\begin{aligned}
 & \left| \int_{\Omega} \phi(\mathbf{x}) \xi(\mathbf{x}, t_{n-1}^c) (\xi(\tilde{\mathbf{x}}_h, t_n^c) - \xi(\tilde{\mathbf{x}}, t_n^c)) d\mathbf{x} \right| \\
 (6.16) \quad & \leq Q \|\xi(\mathbf{x}, t_{n-1}^c)\|_{L^\infty} \|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\| \left(\int_0^1 \int_{\Omega} |\nabla \xi(\tilde{\mathbf{x}} + s(\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}), t_n^c)|^2 d\mathbf{x} ds \right)^{1/2} \\
 & \leq K_1 Q |\ln h_c|^{1/2} \|\xi(\mathbf{x}, t_{n-1}^c)\|_{H^1} \|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\| \|\nabla \xi(\mathbf{x}, t_{n-1}^c)\| \\
 & \leq \varepsilon \Delta t_n^c (\|\nabla \xi(\mathbf{x}, t_n^c)\|^2 + \|\nabla \xi(\mathbf{x}, t_{n-1}^c)\|^2 + \|\xi(\mathbf{x}, t_{n-1}^c)\|^2),
 \end{aligned}$$

provided that

$$(6.17) \quad 2K_1 Q Q_3 h_p^{2q} |\ln h_c|^{1/2} \leq \varepsilon, \quad 2K_1 Q Q_4 h_p^{2q} |\ln h_c|^{1/2} \leq \varepsilon. \quad \square$$

LEMMA 6.5. *Under the conditions of Theorem 5.1, estimate (5.7) holds for $n = N_{m-1} + 1, \dots, N_m$.*

Proof. We decompose the second and seventh terms on the right-hand side of (5.4) as follows:

$$\begin{aligned}
 & \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_n^c) \xi(\mathbf{x}, t_n^c) d\mathbf{x} - \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_{n-1}^c) \xi(\mathbf{x}, t_{n-1}^{c,+}) d\mathbf{x} \\
 (6.18) \quad & = \int_{\Omega} \phi(\mathbf{x}) \left[\int_{t_{n-1}^c}^{t_n^c} \frac{\partial \eta(\mathbf{x}, t)}{\partial t} dt \right] \xi(\mathbf{x}, t_n^c) d\mathbf{x} \\
 & \quad - \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_{n-1}^c) (\xi(\tilde{\mathbf{x}}_h, t_n^c) - \xi(\tilde{\mathbf{x}}, t_n^c)) d\mathbf{x} \\
 & \quad - \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_{n-1}^c) (\xi(\tilde{\mathbf{x}}, t_n^c) - \xi(\mathbf{x}, t_n^c)) d\mathbf{x}.
 \end{aligned}$$

The first term on the right-hand side of (6.18) is bounded by

$$\begin{aligned}
 & \left| \int_{\Omega} \phi(\mathbf{x}) \left[\int_{t_{n-1}^c}^{t_n^c} \frac{\partial \eta(\mathbf{x}, t)}{\partial t} dt \right] \xi(\mathbf{x}, t_n^c) d\mathbf{x} \right| \\
 (6.19) \quad & \leq Q (\Delta t_n^c)^{1/2} \|\xi(\mathbf{x}, t_n^c)\| \|\eta\|_{H^1(t_{n-1}^c, t_n^c; L^2)} \\
 & \leq Q \Delta t_n^c \|\xi(\mathbf{x}, t_n^c)\|^2 + A_1^2 h_c^{2l+2} \|c\|_{H^1(t_{n-1}^c, t_n^c; H^{l+1})}^2.
 \end{aligned}$$

We use (3.15) to bound the third term on the right-hand side of (6.18)

$$\begin{aligned}
 (6.20) \quad & \left| \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_{n-1}^c) (\xi(\tilde{\mathbf{x}}, t_n^c) - \xi(\mathbf{x}, t_n^c)) d\mathbf{x} \right| \\
 &= \left| \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_{n-1}^c) (\tilde{\mathbf{x}} - \mathbf{x}) \cdot \int_0^1 \nabla \xi(\mathbf{x} + s(\tilde{\mathbf{x}} - \mathbf{x}), t_n^c) d\mathbf{x} \right| \\
 &\leq Q \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\| \|\eta(\mathbf{x}, t_{n-1}^c)\| \\
 &\leq \varepsilon \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 + Q \Delta t_n^c h_c^{2l+2} \|c\|_{L^\infty(H^{l+1})}^2.
 \end{aligned}$$

We use the estimate (6.6) with $q = 2(2+\gamma)/\gamma$ and the generalized Hölder inequality to bound the second term on the right-hand side of (6.18) in a similar manner to the estimate of (6.16) as follows:

$$\begin{aligned}
 (6.21) \quad & \left| \int_{\Omega} \phi(\mathbf{x}) \eta(\mathbf{x}, t_{n-1}^c) (\xi(\tilde{\mathbf{x}}_h, t_n^c) - \xi(\tilde{\mathbf{x}}, t_n^c)) d\mathbf{x} \right| \\
 &\leq Q \|\tilde{\mathbf{x}}_h - \tilde{\mathbf{x}}\|_{L^{\frac{2(2+\gamma)}{\gamma}}} \|\eta(\mathbf{x}, t_{n-1}^c)\|_{L^{2+\gamma}} \|\nabla \xi(\mathbf{x}, t_n^c)\| \\
 &\leq \varepsilon \Delta t_n^c \|\nabla \xi(\mathbf{x}, t_n^c)\|^2 + Q \Delta t_n^c h_c^{2l+2} \|c\|_{L^\infty(W_{2+\gamma}^{l+1})}^2,
 \end{aligned}$$

provided that

$$(6.22) \quad QQ_3 h_p^{\frac{\gamma}{2+\gamma}} \leq \varepsilon, \quad QQ_4 h_p^{\frac{\gamma}{2+\gamma}} \leq \varepsilon. \quad \square$$

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