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THE TRANSPORT OF NUCLEAR CONTAMINATION IN FRACTURED POROUS MEDIA

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Abstract. The objects of this paper are to formulate a model for the transport of a chain of radioactive waste products in a fractured porous medium, to devise an effective and efficient numerical method for approximating the solution of the model, and to demonstrate the convergence of the numerical method. The formulation begins from a model in an unfractured (single porosity) medium, passes through a double porosity model in a fractured medium, and ends with a modified single porosity model that takes the relevant time scales of the flow and the nuclear decay.

1. Introduction

We formulate a model for the transport of a chain of radioactive waste products in a fractured porous medium, devise an effective and efficient numerical method for approximating the solution of the model, and demonstrate the convergence of the numerical method. The model is intended to be a reasonably accurate description of the transport and dispersion of nuclear contamination through a granitic medium having densely spaced fractures that are the result of shrinkage; geologic faults are not covered herein. Many nuclear waste facilities are expected to be located in such granitic media.

We begin with a standard model for the transport and dispersion of a nuclear chain in an unfractured, single-porosity porous medium [23] and then introduce a dual porosity model derivable by homogenization. By considering the size of the matrix blocks and the time scale of the problem, we reduce the dual porosity model to a so-called "limit model", which takes the form of a single porosity model with coefficients modified

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to account for the geometry of the fracture system (see [12]) and fluid capacity and nuclear decay within the blocks.

2. The single porosity model

Spagnuolo [23] treated the model to be described below and established its well-posedness, along with a numerical method (the *Modified Method of Characteristics with Adjusted Advection*) for approximating its solution. The model includes an elliptic equation for the pressure and a collection of transport-dominated diffusion equations for the concentrations of the chain of nuclear components.

Assume that the physical system can be described as the miscible flow in an unfractured porous medium of a mixture of a chain of nuclear contaminants with quite low concentrations dissolved in groundwater. We assume that the groundwater is otherwise uncontaminated (or that any other contamination has no effect on the nuclear components or on the flow of the water). We shall also assume that the fluid is incompressible (the effect of compressibility is far smaller than the effects of data uncertainty) and that the concentrations of the contaminants are too small to have a significant effect on the viscosity μ of the fluid. Then, the *pressure equation* is given by Darcy's law and conservation of mass for the total flow for an incompressible single-phase fluid:

$$-\nabla \cdot \left(\frac{1}{\mu} k \nabla p \right) = q, \quad x \in \Omega \subset \mathbf{R}^n, \; n = 2 \text{ or } 3, \tag{2.1}$$

where $k = k(x)$ is the (possibly tensor) permeability of the medium, p is the pressure, and q is the external volumetric flow rate of water (sources and sinks). Gravitational effects will be ignored in the presentation of the modelling process; they will be included when the numerical procedure is introduced. Boundary conditions would need to be specified if we were interested in the single porosity system itself, rather than in it as a means to derive a model in a fractured medium. The associated Darcy velocity is given by

$$\mathbf{u} = \mathbf{u}(x) = -\frac{k}{\mu} \nabla p, \quad x \in \Omega, \; \forall t. \tag{2.2}$$

The *concentration equations* are based on having a chain of N nuclear components, with the $(i-1)^{st}$ component decaying into the i^{th} component. Then, for $i = 1, \dots, N$,

$$\phi r_i \frac{\partial c_i}{\partial t} + \nabla \cdot (c_i \mathbf{u} - D_i \nabla c_i) = \lambda_{i-1}(\phi r_{i-1} c_{i-1}) - \lambda_i(\phi r_i c_i) + \widetilde{c}_i q, \tag{2.3}$$

$$D_i = \phi \left[d_{i,\mathrm{mol}} I + |\mathbf{u}| (d_{i,\mathrm{long}} E(\mathbf{u}) + + d_{i,\mathrm{trans}} E^{\perp}(\mathbf{u}) \right], \tag{2.4}$$

for $x \in \Omega$ and $0 \leq t \leq T$, where $E(\mathbf{u})$ denotes the projection along the vector $\mathbf{u}$ and $E^{\perp}$ its orthogonal complement. Here, ϕ is the porosity of the medium, r_i is the retardation coefficient for the i^{th} component, λ_i the decay constant for the decay from the i^{th} to the $(i+1)^{st}$ component, and D_i the diffusion-dispersion coefficient. Here, $\lambda_0 = r_0 = c_0 = 0$.

3. A dual porosity model

Dual porosity models have been used in a variety of forms for about four decades to describe the flow of fluids in a fractured porous medium. A satisfactory method of deriving a computationally feasible model utilizes the technique of homogenization, given appropriate scalings in the physical properties, to begin from a single porosity model with rapidly varying physical properties that reflect the differences between their values in the fractures and in the unbroken porous stone to obtain a so-called dual porosity model for the fractured medium on a two-sheeted covering of the domain Ω. In this averaging process, the fractures are smeared into one sheet, which consists of a standard Euclidean covering of Ω. The matrix blocks (*i.e.*, the blocks of unfractured porous stone lying between the physical fractures) are replaced by a six-dimensional space $\Omega \times B$ consisting of one (three-dimensional) block B of the same dimensions and characteristics as the original blocks being topologically suspended over each point in the fracture sheet. The topology on $\Omega \times B$ is the product of the discrete topology on Ω by the standard Euclidean topology on B. Then, the model consists of a standard single porosity model on each block, along with another single porosity model on the fracture sheet, though with a permeability tensor modified to take the geometry of the matrix blocks into account. The block B_x over $x \in \Omega$ interacts with the fracture sheet only at the point x, and there only through its boundary ∂B_x, and does not interact directly with the blocks suspended over other points; this is a so-called *totally* fractured medium; it is possible to introduce some interaction between adjacent blocks to obtain a *partially* fractured medium, but this possibility will not be discussed here. The interaction between a block and the fracture sheet will be indicated below. Since we are treating miscible flow and the homogenization procedure has been carried out in detail for this type of flow several times in the literature [7, 11], we shall omit the homogenization derivation and adopt the model that would result.

For conceptual simplicity, gravitational effects will continue to be omitted. Quantities associated with the fracture sheet will usually be indicated by the subscript $_F$, while those associated with blocks will be denoted by the subscript $_B$. The global space variable is x (on Ω) and the local space variable (on a block B_x) is y, so that a point in B_x has the coordinates (x, y). All external flow will be assigned to the fracture sheet.

3.1. Matrix block equations

Consider a matrix block $B = B_{x_B}$ centered over $x_B \in \Omega$. Then, the pressure equation on B is given by

$$\begin{cases} -\nabla_y \cdot \left(\dfrac{k_B}{\mu}\nabla_y p_B\right) = 0, \\ p_B\big|_{\partial B} = p_F\big|_{\partial B}, \end{cases} \tag{3.1}$$

where

$$p_B\big|_{\partial B} = p_F(x_B) + \nabla_x p_F(x_B)\cdot(y - x_B), \quad y \in \partial B. \tag{3.2}$$

Note that the pressure gradient across the block has been retained in the boundary condition; in models of immiscible flow in fractured media, this term is usually ignored, as capillarity is the primary driving force in the displacement process in the blocks. If it were ignored here, the displacement in the blocks would be caused solely by molecular diffusion (as can be seen from the discussion below by killing the $\nabla_x p_F$-term) and would not at all be an accurate representation of the physical process.

Below, we shall specify the boundary and external flow data for the problem on the fracture sheet such that p_F will be independent of t and, consequently, p_B will also be independent of t, though clearly dependent on x_B. Consequently, the Darcy velocity in $B = B_x$ will be given by

$$\mathbf{u}_B = -\frac{k_B}{\mu}\nabla_y p_B, \quad y \in B_x,\ x \in \Omega,\ \forall t. \tag{3.3}$$

The boundary condition expresses the conservation of momentum across ∂B. Conservation of mass will be assured by the source terms in the concentration equations in the fractures that account for the transfer of mass between the blocks and the fractures.

The equations for the concentrations $c_{B,i}$, $i = 1, \dots, N$, are given by

$$\begin{aligned} \phi_B r_{B,i}\frac{\partial c_{B,i}}{\partial t} &+ \nabla_y \cdot (c_{B,i}\mathbf{u}_B - D_{B,i}\nabla_y c_{B,i}) \\ &= \lambda_{i-1}\phi_B r_{B,i-1} c_{B,i-1} - \lambda_i \phi_B r_{B,i} c_{B,i}, \end{aligned} \tag{3.4}$$

along with the boundary conditions

$$c_{B,i}\big|_{\partial B} = c_{F,i}\big|_{\partial B} = c_{F,i}(x_B) + \nabla_x c_{F,i}(x_B) \cdot (y - x_B), \tag{3.5}$$

where the consistency of the composition of the fluid between the fractures and the matrix blocks is expressed by the boundary condition in the system above.

3.2. The equations on the fracture sheet

The flow on the fracture sheet is, as noted earlier, described by a single porosity model of miscible displacement, but with a permeability tensor modified [7] to take into account the geometry of the (still) periodic structure of the medium. The pressure equation takes the form

$$-\nabla_x \cdot \left(\frac{1}{\mu} k_F \nabla_x p_F\right) = q, \quad x \in \Omega,\ 0 \le t \le T, \tag{3.6}$$

with the Darcy velocity in the fractures given by

$$\mathbf{u}_F = -\frac{1}{\mu} k_F \nabla_x p_F. \tag{3.7}$$

In addition, a boundary condition on either p_F or $\mathbf{u}_F$, or one involving both, must be specified on $\partial\Omega$. Assume that both the external flow rate q and the boundary condition are time-invariant; in this case, p_F and $\mathbf{u}_F$ are time-independent.

The tensor k_F is symmetric and positive definite. Its off diagonal terms, in particular, reflect the shape of the blocks. In the two-dimensional case, consider the effect of having $k_{F,11} = k_{F,22}$ and $k_{F,12} = k_{F,21} = \rho k_{F,11}$, where $0 < \rho < 1$. If the boundary conditions would have caused the flow to be in the x-direction if $k_{F,12} = 0$, then the effect of the off diagonal terms is to cause a drift in the positive y-direction as the fluid moves to the right; this corresponds to having the fundamental period in the structure to be a parallelogram with top and bottom parallel to the x-axis and the having its top displaced to the right with respect to the bottom (see Figure 1). Now, in a real granitic domain, both the underlying permeabilities and the shapes of the blocks should be considered as random variables; we shall not address that issue in this paper and shall take it up elsewhere.

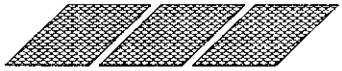

FIGURE 1. An example of three fundamental periods in the special case where the off-diagonal terms of the fracture permeability matrix are of the form $k_{F,11} = k_{F,22}$ and $k_{F,12} = k_{F,21} = \rho k_{F,11}$, where $0 < \rho < 1$.

The concentration equations in the fractures are given by

$$
\begin{aligned}
(3.8)\quad & \phi_F r_{F,i}\frac{\partial c_{F,i}}{\partial t} + \nabla_x \cdot (c_{F,i}\mathbf{u}_F - D_{F,i}\nabla_x c_{F,i}),\\
=&\lambda_{i-1}\phi_F r_{F,i-1}c_{F,i-1} - \lambda_i(\phi_F r_{F,i}c_{F,i}) + \widetilde{c}_{F,i}q_{\text{ext}}\\
&+ \frac{1}{|B_x|}\int_{\partial B_x}(c_{B,i}\mathbf{u}_{B_x} - D_{B,i}\nabla_y c_{B,i})\cdot \nu_B ds.\\
=&\lambda_{i-1}\phi_F r_{F,i-1}c_{F,i-1} - \lambda_i\phi_F r_{F,i}c_{F,i} + \widetilde{c}_{F,i}q_{\text{ext}}\\
&- \frac{\phi_B}{|B_x|}\int_{B_x}\left(\phi_B r_{B,i}\frac{\partial c_{B,i}}{\partial t} + \lambda_i r_{B,i}c_{B,i} - \lambda_{i-1}r_{B,i-1}c_{B,i-1}\right) dy,
\end{aligned}
$$

for $x \in \Omega$, $0 < t \le T$ and $i = 1, \ldots, N$. Boundary conditions must also be specified for the concentrations. Conservation of mass across the ∂B-interfaces is expressed by the integral source terms over B or ∂B, as noted above. All external flow has been assigned to the fracture sheet. The functions $\widetilde{c}_{F,i}$ must be explained. Where fluid is being injected into the domain (where $q > 0$), it is necessary to specify $\widetilde{c}_{F,i}(x)$ as a function of time. When $q < 0$, then what is produced is what is there; *i.e.*, if $q(x) < 0$, then $\widetilde{c}_{F,i}(x,t) = c_{F,i}(x,t)$.

This completes the description of the contaminant transport problem in a fractured medium as a dual porosity system. Clearly, this model is rather complicated; several factors, some physical and some mathematical, allow us to try to capture the main features of the dual porosity model through a somewhat simpler model. The time scale is the primary source for our simplification, since the period of interest is in the hundreds to thousands of years, while the blocks can be expected to be in the scale of at most a few meters; thus, the blocks can be treated as if they were in local equilibrium with the fractures (a "pseudo-stationary" hypothesis) for the purpose of time stepping a numerical calculation in a practical simulation. This will allow us to eliminate calculations in the blocks; moreover, it will then be clear how to generalize the model to permit a non-periodic variation in the physical properties of the medium.

4. Analysis of the solution in the matrix blocks

We need to consider the solution in the blocks over time steps that are reasonable for the fracture sheet. Decompose the pressure on B as follows:

$$p_B = p_F(x_B) + \pi_B(y), \tag{4.1}$$

where

$$\begin{cases} -\nabla_y \cdot \left(\dfrac{k_B}{\mu} \nabla_y \pi_B \right) = 0, \\ \pi_B \big|_{\partial B} = \nabla_x p_F(x_B) \cdot (y - x_B). \end{cases} \tag{4.2}$$

We have assumed the viscosity μ to be constant, and we shall assume now that we can consider the permeabilty k_B to be constant and diagonal on each B. Then, π_B satisfies

$$\begin{cases} \Delta_y \pi_B = 0, \\ \pi_B \big|_{\partial B} = \nabla_x p_F(x_B) \cdot (y - x_B). \end{cases} \tag{4.3}$$

Then, it follows easily that

$$\pi_B = \nabla_x p_F(x_B) \cdot (y - x_B), \quad y \in B, \tag{4.4}$$

and

$$\mathbf{u}_B = -\frac{k}{\mu} \nabla_x p_F(x_B), \tag{4.5}$$

which is independent of y on B_x and of the block size.

Next, let us show that

$$c_{B,i}(y,t) \to c_{F,i}(x_B) + \nabla_x c_{F,i}(x_B) \cdot (y - x_B) \tag{4.6}$$

as the block size tends to zero. This limiting behavior is physically applicable in granite, given the actual block sizes and the time scale of nuclear contamination problems.

Consider the one-dimensional problem; the argument in two or three space variables follows the same lines. Let $B = [-h, h]$; then

$$
\begin{cases}
\phi_B r_{B,i} \dfrac{\partial c_{B,i}}{\partial t} + \dfrac{\partial}{\partial y}(c_{B,i}\mathbf{u}_B - D_{B,i}\nabla_y c_{B,i}) \\
\qquad = \lambda_{i-1}\phi_B r_{B,i-1} c_{B,i-1} - \lambda_i \phi_B r_{B,i} c_{B,i}, \quad -h < y < h, \\
c_{B,i}(-h,t) = c_{F,i}(x_B,t) - h\dfrac{\partial c_{F,i}}{\partial x}(x_B,t), \\
c_{B,i}(h,t) = c_{F,i}(x_B,t) + h\dfrac{\partial c_{F,i}}{\partial x}(x_B,t),
\end{cases}
$$

where

$$D_{B,i} = D_{B,i}(\mathbf{u}_B) = D,$$

a constant tensor on B. Thus,

$$
\begin{aligned}
&\phi_B r_{B,i} \frac{\partial c_{B,i}}{\partial t} + \frac{\partial}{\partial y}(c\mathbf{u}_B - D\frac{\partial c_{B,i}}{\partial y}) \\
&= \phi_B r_{B,i} \frac{\partial c_{B,i}}{\partial t} + \mathbf{u}_B \frac{\partial c_{B,i}}{\partial y} - D\frac{\partial^2 c_{B,i}}{\partial y^2}.
\end{aligned}
$$

Let

$$c_{B,i}(y,t) = c_{F,i}(x_B,t) + y\frac{\partial c_{F,i}}{\partial x}(x_B,t) + \gamma_i(y,t).$$

Then,

$$\gamma_i(-h,t) = \gamma_i(h,t) = 0.$$

So,

$$
\begin{aligned}
&\phi_B r_{B,i} \frac{\partial c_{B,i}}{\partial t} + \mathbf{u}_B \frac{\partial c_{B,i}}{\partial y} - D\frac{\partial^2 c_{B,i}}{\partial y^2} \\
&= \phi_B r_{B,i} \frac{\partial c_{F,i}}{\partial t} + \phi_B r_{B,i} y \frac{\partial^2 c_{F,i}}{\partial x \partial t} + \phi_B r_{B,i} \frac{\partial \gamma_i}{\partial t} + \mathbf{u}_B \frac{\partial c_{F,i}}{\partial x} \\
&\quad + \mathbf{u}_B \frac{\partial \gamma_i}{\partial y} - D\frac{\partial^2 \gamma_i}{\partial y^2} \\
&= \lambda_{i-1}\phi_B r_{B,i-1}\left(c_{F,i-1} + y\frac{\partial c_{F,i-1}}{\partial x} + \gamma_{i-1}\right) \\
&\quad - \lambda_i \phi_B r_{B,i-1}\left(c_{F,i} + y\frac{\partial c_{F,i}}{\partial x} + \gamma_i\right),
\end{aligned}
$$

and

$$\phi_B r_{B,i}\frac{\partial \gamma_i}{\partial t} + \mathbf{u}_B\frac{\partial \gamma_i}{\partial y} - D\frac{\partial^2 \gamma_i}{\partial y^2} + \lambda_i \phi_B r_{B,i}\gamma_i - \lambda_{i-1}\phi_B r_{B,i-1}\gamma_{i-1}$$
$$= -\phi_B r_{B,i}\frac{\partial c_{F,i}}{\partial t} - \phi_B r_{B,i} y\frac{\partial^2 c_{F,i}}{\partial x \partial t} - \mathbf{u}_B\frac{\partial c_{F,i}}{\partial x}$$
$$+ \lambda_{i-1}\phi_B r_{B,i-1}\left(c_{F,i-1} + y\frac{\partial c_{F,i-1}}{\partial x}\right) - \lambda_i \phi_B r_{B,i}\left(c_{F,i} + y\frac{\partial c_{F,i}}{\partial x}\right).$$

Scale the problem by letting $y \to z = h^{-1}y$; thus,

$$\phi_B r_{B,i}\frac{\partial \gamma_i}{\partial t} + \frac{1}{h}\mathbf{u}_B\frac{\partial \gamma_i}{\partial z} - \frac{1}{h^2}D\frac{\partial^2 \gamma_i}{\partial z^2} + \lambda_i \phi_B r_{B,i}\gamma_i - \lambda_{i-1}\phi_B r_{B,i-1}\gamma_{i-1}$$
$$= F + hG,$$

or

$$-D\frac{\partial^2 \gamma_i}{\partial z^2} + h\mathbf{u}_B\frac{\partial \gamma_i}{\partial z} + h^2\phi_B r_{B,i}\frac{\partial \gamma_i}{\partial t} = h^2 H.$$

As $h \to 0$,

$$\frac{\partial^2 \gamma_i}{\partial z^2} \to 0;$$

i.e., $\lim_{h\to 0}\gamma_i$ is linear and vanishes at ± 1, so that $\gamma_i \to 0$ and the desired asymptotic form has been achieved for $c_{B,i}$. Essentially the same argument shows that $\Delta_y \gamma_i \to 0$ in the multidimensional case.

Now,

$$c_{B,i} \sim c_{F,i}(x_B) + \nabla_x c_{F,i}(x_B)\cdot(y - x_B), \quad y \in B, \tag{4.7}$$

implies that

$$\frac{\phi_B}{|B_x|}\int_{B_x}\left(r_{B,i}\frac{\partial c_{B,i}}{\partial z} + \lambda_i r_{B,i}c_{B,i} - \lambda_{i-1}r_{B,i-1}c_{B,i-1}\right)dy \tag{4.8}$$
$$\to \phi_B\left(r_{B,i}\frac{\partial c_{F,i}}{\partial t} - \lambda_{i-1}c_{F,i-1} + \lambda_i r_{B,i}c_{F,i}\right)(x_B, t)$$

as $\mathrm{diam}(B_x) \to 0$.

5. The limit model

Combining (3.8) and (4.8) allows us to eliminate the blocks from the dual porosity model to lead to a modified single porosity system, which we shall call the *limit model* for the transport of a chain of nuclear components in a fractured porous medium; see [12] for a corresponding limit model for immiscible displacement. The limit model here is described by the concentration equations

$$(5.1)\qquad (\phi_F r_{F,i} + \phi_B r_{B,i})\frac{\partial c_{F,i}}{\partial t} + \nabla_x\left(c_{F,i}\mathbf{u}_F - D_{F,i}\nabla_x c_{F,i}\right)$$
$$= \lambda_{i-1}\left(\phi_F r_{F,i-1} + \phi_B r_{B,i-1}\right)c_{F,i-1} - \lambda_i\left(\phi_F r_{F,i} + \phi_B r_{B,i}\right)c_{F,i} + \widetilde{c}_{F,i}q_{ext},$$

for $i = 1, \dots, N$, and the pressure equation (repeating (3.6) and (3.7) in slightly different form)

$$(5.2)\qquad \nabla_x \cdot \mathbf{u}_F = q, \quad \mathbf{u}_F = -\frac{1}{\mu}k_F\nabla_x p_F, \quad x \in \Omega.$$

If reasonable boundary conditions are added to system, such as "no-flow" across $\partial\Omega$, and the coefficients are assumed smooth, then a relatively routine application of energy inequality methods leads to a demonstration of existence, uniqueness, and continuous dependence on the data for solutions of (5.1)-(5.2); see [22] for the general approach and [11] for an analysis of a model of a different type for flow in a fractured medium.

Let

$$r_i^L = \phi_F r_{F,i} + \phi_B r_{B,i},$$

where the superscript ^{L} indicates "limit". For visual clarity, let us simplify the notation by dropping the subscript $_F$, so that $c_{F,i} = c_i$, $i = 1, \dots, N$, $p_F = p$, and $\mathbf{u}_F = u$. Then, introduce the gravitational term into the pressure equation before beginning the numerical treatment of the system and then employ (5.3) to rewrite the concentration equations in the nondivergence form. For $x \in \Omega$ and $t \in J = [0, T]$,

$$(5.3)\qquad u = -\frac{1}{\mu}k(\nabla p + \rho g \nabla d), \quad \nabla \cdot u = q,$$

$$(5.4)\qquad r_i^L\frac{\partial c_i}{\partial t} + u \cdot \nabla c_i - \nabla \cdot (D_i \nabla c_i)$$
$$= -\lambda_i r_i^L c_i + \lambda_{i-1} r_{i-1}^L c_{i-1} + (\widetilde{c}_i - c_i)q^+,$$

$$(5.5)\qquad c_i u \cdot n_\Omega \,|_{\partial\Omega} = (D_i \nabla c_i) \cdot n_\Omega \,|_{\partial\Omega} = 0,$$

$$(5.6)\qquad c_i(x, 0) = c_{i,init}(x),$$

where $q^+ = \max\{q, 0\}$, and $\nabla = \nabla_x$. Note that gravity does not enter the concentration equations.

6. The general simulation problem

We are primarily interested in the interior behavior of the flow process. In order to focus the attention on the interior, we assume $\Omega = [0,1]^d$ and seek Ω-periodic solutions u, p, and c_i. Therefore, the boundary conditions can be dropped. Note that as long as the net exterior flow is zero, the pressure is determined up to an additive constant.

Since the viscosity is independent of the concentrations, the pressure equation is decoupled from the concentration equations; that is, the volumetric flow rate u, which is the only quantity that is passed from the pressure equation to the concentration equations, does not depend on the concentrations of the contaminants and can therefore be computed independently. Indeed, it can be computed in advance of the concentration calculation. If the external flow is held fixed for the duration of the simulation, u can be computed once and used throughout the concentration calculation. Obviously, it would then be inexpensive with respect to the overall calculation to compute u to a very high degree of accuracy. So, we shall assume that the error in u can be ignored in the analysis of the errors in the concentrations, though we shall mention briefly the approximation of (5.3) by mixed finite element methods.

The concentrations will be approximated by a *modified method of characteristics with adjusted advection* procedure [9, 10]; this technique is an improvement over the older *modified method of characteristics* [6, 14, 21] in that the $MMOCAA$ will conserve the mass of each component globally, while the $MMOC$ fails to preserve this highly important physical property.

7. The pressure equation

Assume that the reservoir is a domain in R^2 or R^3. With $\gamma(x) = \rho g \nabla d(x)$ and $a(x) = \mu/k(x)$, multiply the first equation in (5.3) by a test function $v \in V = H_\pi(\operatorname{div}, \Omega)$, the space of Ω-periodic functions in $H(\operatorname{div}, \Omega)$, and integrate over Ω. Then, multiply the second in (5.3) by a test function $w \in W = L^2_{\pi,0}(\Omega)$, the space of Ω-periodic L^2-functions that have mean value zero. Using integration by parts, we see that the weak form of (5.3) is to seek

$$\{u, p\} : J \to V \times W$$

such that

$$(7.1)\qquad (au,v)-(\nabla\cdot v,p)=(\gamma,v),\qquad v\in V,$$
$$(7.2)\qquad (\nabla\cdot u,w)=(q,w),\qquad w\in W.$$

For $h_p>0$, let $P'_{h_p}(\Omega)$ be a quasiregular partition of Ω with elements of diameter bounded by h_p. As in Arbogast [1], we consider $V_{h_p}\times W_{h_p}$ to be one of the approximation spaces of Raviart-Thomas-Nedelec [20, 18], Brezzi-Douglas-Fortin-Marini [4], Brezzi-Douglas-Marini [5] or Brezzi-Douglas-Durán-Fortin [3] associated to the partition and of index such that the approximation properties listed below hold: for any $(v,w)\in H_\pi(\operatorname{div};\Omega)\times L^2_{\pi,0}(\Omega)$,

$$(7.3)\qquad \inf_{\psi\in V}\|v-\psi\|\le Q\|v\|_r h_p^r,\qquad 0\le r\le r^*,$$
$$(7.4)\qquad \inf_{\psi\in V}\|v-\psi\|_{H(\operatorname{div})}\le Q\|v\|_{H^r(\operatorname{div})}h_p^r,\qquad 0\le r\le r^{**},$$
$$(7.5)\qquad \inf_{\varphi\in W}\|w-\varphi\|\le Q\|w\|_r h_p^r,\qquad 0\le r\le r^{**},$$

where $r^{**}=r^*\ge 1$ for the first two spaces [20, 18, 4] and $r^{**}=r^*-1\ge 1$ for the last two [5, 3]. Note also that

$$(7.6)\qquad \|v\|_{L^\infty}\le Q\,h_p^{-1}\|v\|,\quad \|v\|_{W^1_\infty(\mathcal{T})}\le Q\,h_p^{-1}\|v\|_{L^\infty(\mathcal{T})},\quad \mathcal{T}\in P'_{h_p}(\Omega).$$

Let the approximate velocity and pressure, $\{U,P\}\in V_{h_p}\times W_{h_p}$, satisfy

$$(7.7)\qquad (aU,v)-(\nabla\cdot v,P)=(\gamma,v),\qquad v\in V_{h_p},$$
$$(7.8)\qquad (\nabla\cdot U,w)=(q,w),\qquad w\in W_{h_p},$$

and set $\theta=p-P$ and $Y=u-U$. Then, the following lemma holds [4, 5, 3, 13].

LEMMA 7.1.

$$(7.9)\qquad \|Y\|_0\le Q\|u\|_r h_p^r,\qquad 1\le r\le r^*,$$
$$(7.10)\qquad \|\nabla\cdot Y\|_0\le Q\|\nabla\cdot u\|_r h_p^r,\qquad 0\le r\le r^{**},$$
$$(7.11)\qquad \|\theta\|_0\le Q\,(\|p\|_r+\|u\|_r)\,h_p^r,\qquad 0\le r\le r^{**}.$$

Note that (U,P) will be computed only at discrete times.

8. A modified method of characteristics with adjusted advection for the concentration equations

The *MMOCAA* is a time-stepping procedure that can be combined with any spatial discretization. We apply this method to (5.4) assuming the velocity is known.

The weak form of the concentration equations is, for $i = 1, \dots, N_c$, to find a map $c_i : J \to H^1_\pi(\Omega)$, where $H^1_\pi(\Omega)$ is the space of Ω-periodic functions in $H^1(\Omega)$, such that

$$\begin{aligned}(8.1)\qquad &\left(r_i^L \frac{\partial c_i}{\partial t} + u \cdot \nabla c_i, \chi\right) + (D_i(u)\nabla c_i, \nabla\chi) \\ &= (-\lambda_i r_i^L c_i + \lambda_{i-1} r_{i-1}^L c_{i-1}, \chi) + ((\widetilde{c}_i - c_i)q, \chi), \quad \chi \in H^1_\pi(\Omega).\end{aligned}$$

The central concept in the standard *MMOC* [21, 14, 1] is to view the hyperbolic part of (5.4) given by $r_i^L \partial c_i/\partial t + u \cdot \nabla c_i$ as a directional derivative. Accordingly, if

$$(8.2)\qquad \Psi_i(x) \equiv \sqrt{(r_i^L)^2 + |u(x)|^2},$$

then

$$(8.3)\qquad \Psi_i \frac{\partial c_i}{\partial \tau_i} = r_i^L \frac{\partial c_i}{\partial t} + u \cdot \nabla c_i,$$

where τ_i is the unit vector $(u_1, u_2, r_i^L)/\Psi_i(x)$, and (5.4) can be written as

$$(8.4)\qquad \Psi_i \frac{\partial c_i}{\partial \tau_i} - \nabla \cdot (D_i(u)\nabla c_i) = (\widetilde{c}_i - c_i)q^+ - \lambda_i r_i^L c_i + \lambda_{i-1} r_{i-1}^L c_{i-1}.$$

Since (8.4) is in the form of the heat equation, its numerical approximations should behave better than those of (5.4) if the directional derivative $\partial c_i/\partial \tau_i$ is treated properly.

Let J be partitioned into $0 = t^0 < t^1 < \cdots < t^N = T$, where $\Delta t_c = t^{n+1} - t^n$ is constant, and let $J_{n+1} = (t^n, t^{n+1})$. Below, we follow [9, 10] to describe the *MMOCAA* mass-conserving technique for our problem, first considering a discretization in the time variable while leaving the spatial variable continuous.

For a function φ on $\Omega \times J$, set $\varphi^n(x) = \varphi(x, t^n)$. Then, approximate the τ_i-derivative by a backward difference quotient; then,

$$(8.5)\qquad \Psi_i(x) \frac{\partial c_i^{n+1}}{\partial \tau_i}(x) \approx r_i^L \frac{c_i^{n+1}(x) - c_i^n(\overline{x}_i)}{\Delta t_c},$$

where

$$\overline{x}_i = x - u(x)\Delta t_c / r_i^L(x). \tag{8.6}$$

For notational convenience, let $\overline{c}_i(x) = c_i(\overline{x}_i)$ (and, later, $\overline{C}_i(x) = C_i(\overline{X}_i)$). Since the problem is Ω-periodic, $\overline{c}_i$ is always defined. Applying (8.5) to (8.4) gives

$$\begin{aligned} r_i^L \frac{c_i^{n+1} - \overline{c}_i^n}{\Delta t_c} &- \nabla \cdot (D_i(u)\nabla c_i) \\ &= (\widetilde{c}_i - c_i)q^+ - \lambda_i r_i^L c_i + \lambda_{i-1} r_{i-1}^L c_{i-1}. \end{aligned} \tag{8.7}$$

Now, integrating (8.7) over $\Omega \times J_{n+1}$ and using periodicity gives

$$\begin{aligned} \int_\Omega r_i^L c_i^{n+1} dx &- \int_\Omega r_i^L \overline{c}_i^n \, dx \\ &= \int_{t^n}^{t^{n+1}} \int_\Omega (\widetilde{c}_i - c_i) q^+ \, dx\, dt \\ &\quad - \int_{t^n}^{t^{n+1}} \int_\Omega (\lambda_i r_i^L c_i - \lambda_{i-1} r_{i-1}^L c_{i-1}) \, dx\, dt. \end{aligned} \tag{8.8}$$

On the other hand, integrating the original equation over $\Omega \times J_{n+1}$ gives

$$\begin{aligned} &\int_\Omega r_i^L c_i^{n+1} dx - \int_\Omega r_i^L c_i^n \, dx \\ &= \int_{t^n}^{t^{n+1}} \int_\Omega \widetilde{c}_i q \, dx\, dt - \int_{t^n}^{t^{n+1}} \int_\Omega (\lambda_i r_i^L c_i - \lambda_{i-1} r_{i-1}^L c_{i-1}) \, dx\, dt. \end{aligned} \tag{8.9}$$

Therefore, in order for mass to be conserved, we must have

$$\begin{aligned} \int_\Omega r_i^L \overline{c}_i^n dx &+ \int_{t^n}^{t^{n+1}} \int_\Omega (\widetilde{c}_i - c_i^{n+1}) q^+ \, dx\, dt \\ &= \int_{t^n}^{t^{n+1}} \int_\Omega \widetilde{c}_i q \, dx\, dt + \int_\Omega r_i^L c_i^n \, dx. \end{aligned} \tag{8.10}$$

Viewing the concentrations over J_{n+1} as being evaluated at time t^{n+1} gives the following discrete form of conservation of mass:

$$\begin{aligned} \int_\Omega r_i^L \overline{c}_i^n dx &+ \Delta t_c \int_\Omega (\widetilde{c}_i^{n+1} - c_i^{n+1}) q^{+,n+1} \, dx \\ &= \Delta t_c \int_\Omega \widetilde{c}_i^{n+1} q^{n+1} \, dx + \int_\Omega r_i^L c_i^n dx. \end{aligned} \tag{8.11}$$

Let

$$\overline{Q}_i^n = \int_\Omega r_i^L \overline{c}_i^n dx. \tag{8.12}$$

Then, with $q^- = \max\{-q, 0\}$ so that $q = q^+ - q^-$,

$$\begin{aligned} &\widetilde{c}_i^{n+1} q^{n+1} - \widetilde{c}_i^{n+1} q^{+,n+1} + c_i^{n+1} q^{+,n+1} \\ &= -\widetilde{c}_i^{n+1} q^{-,n+1} + c_i^{n+1} q^{+,n+1} = c_i^{n+1} q^{n+1}. \end{aligned} \tag{8.13}$$

Using (8.12) and (8.13), we can write the semi-discrete conservation of mass equation as

$$\overline{Q}_i^n = Q_i^n, \tag{8.14}$$

where

$$Q_i^n \equiv \int_\Omega r_i^L c_i^n dx + \Delta t_c \int_\Omega c_i^{n+1} q^{n+1}\, dx. \tag{8.15}$$

Since c_i^{n+1} is the unknown at this time step, we define an extrapolation $E(\Delta t)\varphi$ by

$$E(\Delta t)\varphi(t) \equiv 2\varphi(t - \Delta t) - \varphi(t - 2\Delta t). \tag{8.16}$$

Then, interpret the second integral in (8.15) to be

$$\Delta t_c \int_\Omega E(\Delta t_c) c_i(t^{n+1}) q^{n+1}\, dx. \tag{8.17}$$

For some fixed $\kappa > 0$, let

$$\begin{cases} x_i^+ = x - \dfrac{u(x)}{r_i^L}\Delta t_c + \kappa \dfrac{u(x)}{r_i^L}(\Delta t_c)^2, \\ x_i^- = x - \dfrac{u(x)}{r_i^L}\Delta t_c - \kappa \dfrac{u(x)}{r_i^L}(\Delta t_c)^2. \end{cases} \tag{8.18}$$

Also, let

$$\overline{c}_i^{\#n} = \begin{cases} \max\{c_i(x_i^+, t^n), c_i(x_i^-, t^n)\} & \text{if } \overline{Q}_i^n \le Q_i^n, \\ \min\{c_i(x_i^+, t^n), c_i(x_i^-, t^n)\} & \text{if } \overline{Q}_i^n > Q_i^n. \end{cases} \tag{8.19}$$

Set

$$\overline{Q}_i^{\#n} \equiv \int_\Omega r_i^L \overline{c}_i^{\#n} dx. \tag{8.20}$$

Now, if $\overline{Q}_i^{\#n} = \overline{Q}_i^n$, then let $\widehat{c}^n \equiv \overline{c}^n$; in this case, we have to accept that mass is not conserved on this time step (this has never happened in any $MMOCAA$ calculation). Otherwise, find $\theta_i^n \in \mathbf{R}$ such that

$$Q_i^n = \theta_i^n \overline{Q}_i^n + (1 - \theta_i^n)\overline{Q}_i^{\#n}, \tag{8.21}$$

and set

$$\widehat{c}_i^n = \theta_i^n \overline{c}_i^n + (1-\theta_i^n)\overline{c}_i^{\#n}. \tag{8.22}$$

Clearly,

$$\int_\Omega r_i^L \widehat{c}_i^n dx = Q_i^n, \tag{8.23}$$

so that mass is conserved globally in space at each time level up to the truncation error introduced by the replacement of double integrals over $\Omega \times [t^n, t^{n+1}]$. Our *MMOCAA* procedure uses $\widehat{c}_i^n$ as the transported concentration in the fractional step procedure in splitting transport and diffusion.

Next, we combine this time discretization scheme with a standard Galerkin procedure in the spatial variables. For $h_c \in (0,1]$, assume that we have a quasi-regular partition $P_{h_c}(\Omega)$ of Ω into simplices or rectangles of diameters bounded by h_c. Let $M_{h_c} \subset W_\infty^1(\Omega)$ be a family of standard Galerkin finite element spaces having the following approximation and inverse properties:

$$\inf_{\chi \in M_{h_c}} [\|f-\chi\| + h_c\|f-\chi\|_1] \le Q_0 h_c^s \|f\|_s, \qquad 1 \le s \le s^*, \tag{8.24}$$

and, for $\chi \in M_{h_c}$

(8.25)

$$\|\chi\|_{W_\infty^1} \le Q_0 h_c^{-1}\|\chi\|_1, \quad d\|\chi\|_{L^\infty} \le Q_0 h_c^{-1}\|\chi\|, \quad \|\chi\|_1 \le Q_0 h_c^{-1}\|\chi\|,$$

where Q_0 is independent of h_c.

9. The computational algorithm

Here, we present a detailed treatment of the computational algorithm to be associated with the concepts of the previous two sections. Since the method can be applied to a number of similar physical problems, we shall not make the simplifying assumption that the Darcy velocity be computed only once. We shall employ possibly different time steps for the pressure and the concentrations.

Partition J into pressure time steps $0 = t_0 < t_1 < \cdots < t_M = T$, with $\Delta t_p^m = t_m - t_{m-1}$, and require that each pressure time step be also a concentration time step; that is, for each $m > 0$, there exists n_m such that $t_m = t^{m-1,n_m}$, where $t^{m,n} = t_m + n\Delta t_c$. Note that superscripts will be used for concentration time steps and subscripts for pressure time steps. Let $\Delta t_c = t^{m,n} - t^{m,n-1}$ be constant. It is usual to have the pressure time step larger than the concentration time step, except possibly for the first few steps.

Recall that the pressure and Darcy velocity are independent of the concentrations of the contaminants and can be evaluated at a time t_{m+1} ahead of the time currently being considered in the concentration calculation. Let $J_{m+1} = (t_m, t_{m+1}]$ and $J_{m,n+1} = (t_{m,n}, t_{m,n+1}]$. If $t^{m,n} \in J_{m+1}$, approximate the Darcy velocity at $t_{m,n}$ by

$$IU^{m,n} = \left(1 - \frac{t^{m,n} - t_m}{t_{m+1} - t_m}\right) U_m + \left(\frac{t^{m,n} - t_m}{t_{m+1} - t_m}\right) U_{m+1}. \tag{9.1}$$

The time-stepping procedure consists of computing maps

$$C_i : \{t^0, \ldots, t^{M-1,n_m} = t_M\} \rightarrow M_{h_c}, \quad i = 1, \ldots, N, \tag{9.2}$$

$$(U, P) : \{t_0, \ldots, t_M\} \rightarrow V \times W, \tag{9.3}$$

as follows:

- **The initial condition:** Find $C_i^0 \in M_{h_c}$ such that

$$(\nabla C_i^0, \nabla v) + (C_i^0, v) = (\nabla c_{i,init}, \nabla v) + (c_{i,init}, v), \qquad v \in M_{h_c}. \tag{9.4}$$

- **The pressure step:** If $m = -1$ or $q_{m+1} \neq q_m$, find $(U_{m+1}, P_{m+1}) \in V_{h_p} \times W_{h_p}$ such that

$$(aU_{m+1}, v) - (\nabla \cdot v, P_{m+1}) = (\gamma, v), \qquad v \in V, \tag{9.5}$$

$$(\nabla \cdot U_{m+1}, w) = (q_{m+1}, w), \qquad w \in W. \tag{9.6}$$

  (If $q_{m+1} = q_m$, just set $(U_{m+1}, P_{m+1}) = (U_m, P_m)$.)
- **The transport fractional step:** Given (U_{m+1}, P_{m+1}), find $C_i^{m,n+1}$ for $i = 1, \ldots, N$, and $n = 0, \ldots, n_m - 1$, such that $t^{m,n_{m+1}} = t_{m+1}$, in the following way:
  1. Given $C_i^{m,n}$ and

$$Q_i^{m,n} = \int_\Omega r_i^L c_i^{m,n} dx + \Delta t_c \int_\Omega E(\Delta t_c) c_i(t^{m,n+1}) q(t^{m,n+1})\, dx,$$

let

$$\overline{x}_i = \overline{x}_i(x) = x - \frac{IU^{m,n+1}(x)}{r_i^L} \Delta t_c, \tag{9.7}$$

$$\overline{C}_i^{m,n}(x) = C_i^{m,n}(\overline{x}_i), \tag{9.8}$$

$$\overline{Q}_i^{m,n} = \int_\Omega r_i^L \overline{C}_i^{m,n}(x) dx. \tag{9.9}$$

If $\overline{Q}_i^{m,n} = Q_i^{m,n}$, then set $\widehat{C}_i^{m,n} = \overline{C}_i^{m,n}$ and go to the diffusive fractional step.

2. If $\overline{Q}_i^{m,n} \neq Q_i^{m,n}$, let

$$\delta_i = \delta_i(x) = \kappa \frac{IU^{m,n+1}}{r_i^L}(\Delta t_c)^2, \tag{9.10}$$

$$x_i^+ = x_i^+(x) = \overline{x}_i + \delta_i, \quad x_i^- = x_i^-(x) = \overline{x}_i - \delta_i, \tag{9.11}$$

$$\overline{C}_i^{\#m,n}(x) = \begin{cases} \max\{C_i^{m,n}(x_i^+), C_i^{m,n}(x_i^-)\} & \text{if } Q_i^{m,n} \geq \overline{Q}_i^{m,n}, \\ \min\{C_i^{m,n}(X_i^+), C_i^{m,n}(X_i^-)\} & \text{if } Q_i^{m,n} < \overline{Q}_i^{m,n}, \end{cases} \tag{9.12}$$

$$\overline{Q}_i^{\#m,n} = \int_\Omega r_i^L \overline{C}_i^{\#m,n}(x)dx. \tag{9.13}$$

3. If $\overline{Q}_i^{m,n} = \overline{Q}_i^{\#m,n}$, then set

$$\widehat{C}_i^{m,n} = \overline{C}_i^{m,n}; \tag{9.14}$$

otherwise, find $\theta_i^{m,n} \in \mathbf{R}$ such that

$$Q_i^{m,n} = \theta_i^{m,n}\overline{Q}_i^{m,n} + (1 - \theta_i^{m,n})\overline{Q}_i^{\#m,n} \tag{9.15}$$

and set

$$\widehat{C}_i^{m,n}(x) = \theta_i^{m,n}\overline{C}_i^{m,n} + (1 - \theta_i^{m,n})\overline{C}_i^{\#m,n}. \tag{9.16}$$

- **The diffusive fractional step:** Recall that $C_0 = r_0 = \lambda_0 = 0$. Find first $C_1^{m,n+1} \in M_{h_c}$, then $C_2^{m,n+1} \in M_{h_c}, \ldots$, and finally $C_N^{m,n+1} \in M_{h_c}$, such that, for $i = 1, \ldots, N$, each $C_i^{m,n+1}$ satisfies

(9.17)

$$\left(r_i^L \frac{C_i^{m,n+1} - \widehat{C}_i^{m,n}}{\Delta t_c}, \chi \right) + \left(D_i(IU^{m,n+1})\nabla C_i^{m,n+1}, \nabla\chi \right)$$
$$= \left(q^{+,m,n+1}\left(\widetilde{c}_i^{m,n+1} - E(\Delta t_c)C_i^{m,n+1} \right), \chi \right)$$
$$+ \left(-\lambda_i r_i^L E(\Delta t_c) C_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \chi \right), \quad \chi \in M_{h_c}, \quad n \geq 1.$$

In the procedure above, we solve first for $C_{i,0}$ for $i = 1, \ldots, N$, then for (U_0, P_0) and (U_1, P_1). The general step proceeds as follows. Given (U_m, P_m), (U_{m+1}, P_{m+1}), and $C_i^{m,n}$, $i = 1, \ldots, N$, compute, in increasing order in i, $C_i^{m,n+1}$. When $t^{m,n+1} = t_{m+1}$, compute (U_{m+2}, P_{m+2}), and replace $m+1$ by m and continue.

Conservation of mass in (9.17) depends on some evaluation of C_i at the unknown time in question. In order to get by with only one solution of an elliptic problem each time step, we chose to use an extrapolation (see (8.17)) to compute this term. Alternatively, we could have chosen to solve for this term implicitly, but this would require an additional elliptic solve in order to conserve mass; see Section 14 for details. Since the new values for $C_{i-1}^{m,n+1}$ are already known when the equation for $C_i^{m,n+1}$ is being solved, it is not necessary to use an extrapolation of C_{i-1}.

10. Technical matter

The regularity assumptions below on the coefficients and solution of (5.3) and (5.4) will be used in the convergence analysis; the formulation of the model is applicable under weaker assumptions. The convergence analysis can also be given under assumptions that the solution is globally in H^1 but piecewise smoother if the partition includes all interfaces across which only the reduced regularity holds. For the Ω-periodic solution $\{c_i, u, p\}$, assume that

$$\text{(A)} \qquad \begin{cases} \text{For} \quad i = 1, \dots, N, \qquad 1 \le r \le r^*, \quad 2 \le s \le s^*, \\ c_i \in L^\infty(H^s) \cap H^1(H^s) \cap L^\infty(W^1_\infty) \cap H^2(L^2), \\ p \in L^\infty(H^r), \\ u \in L^\infty(H^r(\operatorname{div})) \cap L^\infty(W^1_\infty) \cap W^1_\infty(L^\infty) \cap H^2(L^2). \end{cases}$$

At first glance, it may seem strange that u, which depends on ∇p, should be required to have more regularity than p. However, this is reasonable, because in the physical problem, the coefficient k/μ may be rough or even discontinuous, particularly at interfaces between different rock types. If k is discontinuous, then ∇p will also be discontinuous, but both the physical p and the physical u should still be continuous there.

The assumptions on the coefficients in the differential equations are as follows:

$$\text{(B)} \qquad \begin{cases} 0 < a_* \le \dfrac{k(x)}{\mu} \le a^*, \quad 0 < \phi_* \le \phi \le \phi^*, \quad 0 < D_* \le D_i(x, u), \\ |\nabla \phi(x)| + \left| \dfrac{\partial D_i}{\partial u}(x, u) \right| + |q(x,t)| + \left| \dfrac{\partial q}{\partial t}(x,t) \right| \le K^*. \end{cases}$$

Each of these assumptions is reasonable given the problem at hand, except maybe that of the source term q, which at a practical computational length scale could contain point sources or sinks.

Following [24] and [8], for our convergence analysis we define appropriate projections of the exact concentrations c_i, for $i = 1, \dots, N$, into

M_{h_c}. With u as the exact Darcy velocity, define $C_i^\dagger : J \to M_{h_c}$ for $i = 1, \ldots, N$, to be the projection of c_i given by

$$\begin{aligned}
&\Big(D_i(u(t))\nabla C_i^\dagger(t), \nabla\chi\Big) + \Big((q^+ + \gamma_0)C_i^\dagger(t), \chi\Big) \\
(10.1) \qquad &= (D_i(u(t))\nabla c_i(t), \nabla\chi) + \big((q^+ + \gamma_0)c_i(t), \chi\big) \\
&= -\left(r_i^L \frac{\partial c_i}{\partial t}(t) + u \cdot \nabla c_i(t), \chi\right) \\
&\quad + \big(-\lambda_i r_i^L c_i(t) + \lambda_{i-1} r_{i-1}^L c_{i-1}(t), \chi\big) \\
&\quad + (q^+(t)\widetilde{c}_i(t), \chi) + (\gamma_0 c_i, \chi), \quad \chi \in M_{h_c}, \quad t \in J,
\end{aligned}$$

where $\gamma_0 > 0$, a constant, and the last equality above follows from (8.1). The following facts about $C_i^\dagger$ are standard results from the analyses of Galerkin methods, so long as both q and its derivative are smooth functions in the spatial variables:

$$(10.2) \qquad \|c_i - C_i^\dagger\|_{L^2} + h_c\|c_i - C_i^\dagger\|_{H^s} \le Q_1 h_c^s \|c_i\|_{H^s}, \quad 1 \le s \le s^*,$$

$$(10.3) \qquad \left\|\frac{\partial}{\partial t}(c_i - C_i^\dagger)\right\|_{L^2(L^2)} \le Q_1 h_c^s \|c_i\|_{H^1(H^s)}, \quad 1 \le s \le s^*,$$

$$(10.4) \qquad \|C_i^\dagger\|_{L^\infty(W^1_\infty)} \le Q_2,$$

where Q_1 is independent of c_i and h_c but depends on $\|u\|_{W^1_\infty(L^\infty)}$ and D_*.

The convergence analysis will rely on estimates of various norms of $C_i - C_i^\dagger$, where C_i is the numerical solution defined above. We shall make use also of the analogue of $\overline{x}_i$ defined for the exact velocity $u^{m,n}$. For a function f on $\Omega \times J$, set (with $+$ or $-$ chosen appropriately)

$$\begin{aligned}
&\overset{\vee}{\overline{x}}_i = x - \frac{Iu^{m,n+1}}{r_i^L}\Delta t_c, \qquad \overset{\vee}{\overline{f}}{}_i^{m,n}(x) = f_i(\overset{\vee}{\overline{x}}_i), \\
&\overset{\vee}{\overline{f}}{}_i^{\#m,n}(x) = f_i\left(\overline{x}_i \pm \kappa \frac{Iu^{m,n+1}}{r_i^L}(\Delta t_c)^2\right) = f(\overset{\vee}{\overline{x}}{}_i^{\pm}), \\
&\overset{\vee}{f}{}_i^{m,n}(x) = \theta_i^{m,n}\, \overset{\vee}{\overline{f}}{}_i^{m,n}(x) + (1 - \theta_i^{m,n})\, \overset{\vee}{\overline{f}}{}_i^{\#m,n}(x).
\end{aligned}$$

The analogous notation with $\widehat{\ }$ replacing $^\vee$ will be used for $\widehat{\overline{x}}_i = x - \dfrac{IU^{m,n+1}}{r_i^L}\Delta t_c, \ldots$, where the approximation U replaces u above. If the notation would produce a variable with a recursive i-subscript, only one will be written.

11. A priori error estimates

In this section, we prove that the *MMOCAA* approximation converges at the optimal rate in $L^2(\Omega)$ to the exact concentration under the above assumptions. Throughout the analysis, we denote by Q and ε generic positive constants, normally large and small, respectively.

The following two theorems are the main convergence results. Theorem 11.1 is a consequence of inequality (11.41). Theorem 11.2 is simply a restatement of part of Lemma 7.1.

THEOREM 11.1. *Let*

$$\begin{aligned}\mathcal{E}_i = \Bigg[& \left(\left\| \frac{\partial^2 c_i}{\partial \tau_{I_i}^2} \right\|_{L^2(L^2)} + \left\| \frac{\partial c_i}{\partial t} \right\|_{L^2(L^2)} \right) \Delta t_c \\ & + \|u_{tt}\|_{L^2(L^2)} (\Delta t_p)^2 + \|u\|_{L^\infty(W^1_\infty)} \|c_i\|_{L^\infty(H^1)} (\Delta t_c)^{3/2} \\ & + \|u\|_{L^\infty(H^r)} h_p^r + \left(\|c_i\|_{L^\infty(H^s)} + \|c_i\|_{H^1(H^s)} \right) h_c^s \Bigg],\end{aligned} \tag{11.1}$$

where τ_{I_i} *will be defined below in* (11.13). *Assume that*

$$\Delta t_c = o(h_p) \quad \text{and} \quad h_p = O(h_c)$$

as the discretization parameters tend to zero and $\max_{i=1,\dots,N} \{\max_{m,n} |\theta_i^{m,n}|\} \leq M$ *for some* $M > 0$. *Then, for* $1 \leq r \leq r^*$ *and* $2 \leq s \leq s^*$, *the following estimate holds asymptotically:*

$$\max_{m,n} \{ \|c_i^{m,n} - C_i^{m,n}\|_0 + \|u^m - U^m\|_0 \} \leq Q\mathcal{E}, \text{ where } \mathcal{E} = \sum_{i=1}^{N} \mathcal{E}_i. \tag{11.2}$$

THEOREM 11.2. *For any* $r \in [0, r^{**}]$,

$$\max_m \|\nabla \cdot (u_m - U_m)\|_0 \leq Q \|\nabla \cdot u\|_{L^\infty(H^r)} h_p^r. \tag{11.3}$$

The proof of Theorem 11.1 will be broken down into several lemmas.

LEMMA 11.1. *Let* $C_i \in L^\infty(0, T; H^1(\Omega))$ *be* Ω*-periodic. Let*

$$\check{C}_i^{m,n} = C_i(\check{\bar{x}}_i, t^{m,n}) \text{ and } \check{C}_i^{\#m,n} = C_i(\check{x}_i^*, t^{m,n}),$$

where $\overset{\vee}{x}{}_i^* = \overset{\vee}{x}{}_i^{*,m,n}(x) = \overset{\vee}{x}{}_i^+(x)$ *or* $\overset{\vee}{x}{}_i^-(x)$ *is given in terms of the interpolation* $Iu^{m,n}$. *Then,*

$$\left\| \overset{\vee}{C}{}_i^{\#m,n} - \overset{\vee}{C}{}_i^{m,n} \right\|_0 \leq Q(\Delta t_c)^2 \|u\|_{L^\infty(W^1_\infty)} \|C_i^{m,n}\|_1. \tag{11.4}$$

Proof. Let z be the unit vector in the direction $u^{m,n+1}(x)/(r_i^L(x))$. Then,

$$\begin{aligned} &(\overset{\vee}{C}{}_i^{\#m,n} - \overset{\vee}{C}{}_i^{m,n})(x) \\ &= \int_0^1 \frac{\partial C_i^{m,n}}{\partial z} \left(\overset{\vee}{\overline{x}}{}_i \pm s\,\kappa \frac{Iu^{m,n+1}}{r_i^L} (\Delta t_c)^2 \right) \frac{\kappa (\Delta t_c)^2}{r_i^L} Iu^{m,n+1} \cdot z\, ds. \end{aligned} \tag{11.5}$$

Squaring both sides and integrating over Ω gives

$$\| \overset{\vee}{C}{}_i^{\#m,n} - \overset{\vee}{C}{}_i^{m,n} \|_0^2 \leq Q\,(\Delta t_c)^4 \|u\|^2_{L^\infty(W^1_\infty)} \|\nabla C_i^{m,n}\|_0^2, \tag{11.6}$$

since the Jacobian of the map $x \mapsto \overset{\vee}{\overline{x}}{}_i \pm s\,\kappa \frac{Iu^{m,n+1}}{r_i^L} (\Delta t_c)^2$, given by $G_s(x) = x - \frac{Iu^{m,n+1}}{r_i^L} \Delta t_c \pm s\kappa \frac{Iu^{m,n+1}}{r_i^L} (\Delta t_c)^2$, is the identity matrix plus Δt_c or $(\Delta t_c)^2$ times terms involving first partial derivatives of $Iu^{m,n+1}$ and ϕ (which are bounded) and $G_s(x)$ is globally at most finitely-many-to one as can be seen in [15] and [21]. So, the lemma follows.

We now let $\xi_i^{m,n} = C_i^{\dagger,m,n} - C_i^{m,n}$, then subtract (9.17) evaluated at time $t^{m,n+1}$ from (10.1) evaluated at time $t^{m,n+1}$, and let $\chi = \xi_i^{m,n+1}$. The following equation, whose derivation can be found in §13, is obtained after some manipulation:

(11.7)

$$\left(r_i^L \frac{\xi_i^{m,n+1}-\xi_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) + \left(D_i(IU^{m,n+1})\nabla\xi_i^{m,n+1}, \nabla\xi_i^{m,n+1}\right)$$

$$\begin{aligned}
= & -\left(\left[D_i(u^{m,n+1}) - D_i(IU^{m,n+1})\right]\nabla C_i^{\dagger,m,n+1}, \nabla\xi_i^{m,n+1}\right) \\
& -\left(r_i^L\left(\frac{c_i^{m,n+1}-c_i^{m,n}}{\Delta t_c} - \frac{C_i^{\dagger,m,n+1}-C_i^{\dagger,m,n}}{\Delta t_c}\right), \xi_i^{m,n+1}\right) \\
& -\left((u^{m,n+1} - Iu^{m,n+1})\cdot\nabla c_i^{m,n+1}, \xi_i^{m,n+1}\right) \\
& -\left(\left[r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + Iu^{m,n+1}\cdot\nabla c_i^{m,n+1}\right] - r_i^L \frac{c_i^{m,n+1} - \check{c}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
& +\left(r_i^L \frac{(\check{c}_i - \check{C}^\dagger{}_i)^{m,n} - (c_i - C_i^\dagger)^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
& +\left(r_i^L \frac{\check{\xi}_i^{m,n} - \xi_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
& -\left(r_i^L \frac{\widehat{C^\dagger}_i^{m,n} - \check{C}^\dagger{}_i^{,m,n}}{\Delta t_c}, \xi_i^{m,n}\right) + \left(r_i^L \frac{\widehat{\xi}_i^{m,n} - \check{\xi}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
& +\left(\lambda_{i-1} r_{i-1}^L (c_{i-1}^{m,n+1} - C_{i-1}^{\dagger,m,n+1}), \xi_i^{m,n+1}\right) + (\lambda_{i-1} r_{i-1}^L \xi_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
& + (q^+ E(\Delta t_c) C_i^{m,n+1}, \xi_i^{m,n+1}) + (\gamma_0 (c_i^{m,n+1} - C_i^{\dagger,m,n+1}), \xi_i^{m,n+1}) \\
& +\left(\lambda_i r_i^L (E(\Delta t_c) C_i^{m,n+1} - c_i^{m,n+1}), \xi_i^{m.n+1}\right) - (q^+ C_i^{\dagger,m,n+1}, \xi_i^{m,n+1}).
\end{aligned}$$

The left-hand side can be bounded below in the following way:

(11.8)

$$\left(r_i^L \frac{\xi_i^{m,n+1}-\xi_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) + \left(D_i(IU^{m,n+1})\nabla\xi_i^{m,n+1}, \nabla\xi_i^{m,n+1}\right)$$

$$\geq \frac{1}{2\Delta t_c}\left[(r_i^L \xi_i^{m,n+1}, \xi_i^{m,n+1}) - (r_i^L \xi_i^{m,n}, \xi_i^{m,n})\right] + K_i \|\nabla\xi_i^{m,n+1}\|_0^2$$

where K_i is a positive constant that depends on i.

The right-hand side of (11.7) will be dealt with next. A routine calculation shows that

$$\|u^{m,n+1} - Iu^{m,n+1}\|_0^2 \leq \|u_{tt}\|^2_{L^2(J_{m+1},L^2)}(\Delta t_p)^3; \tag{11.9}$$

hence,

$$\|u^{m,n+1} - IU^{m,n+1}\|_0^2 \leq Q\|u_{tt}\|^2_{L^2(J_{m+1},L^2)}(\Delta t_p)^3 + \|IY^{m,n+1}\|_0^2. \tag{11.10}$$

Together (11.9) and (11.10) can be used to handle the first and third terms as follows:

$$\begin{aligned}
&-\left(\left[D_i(u^{m,n+1}) - D_i(IU^{m,n+1})\right]\nabla C_i^{\dagger,m,n+1}, \nabla\xi_i^{m,n+1}\right) \\
&\quad - \left((u^{m,n+1} - Iu^{m,n+1})\cdot\nabla c_i^{m,n+1}, \xi_i^{m,n+1}\right) \\
&\leq Q\left\{\|u_{tt}\|^2_{L^2(J_{m+1};L^2)}(\Delta t_p)^3 + \|IY^{m,n+1}\|_0^2 + \|\xi_i^{m,n+1}\|_0^2\right\} \\
&\quad + \varepsilon\|\nabla\xi_i^{m,n+1}\|_0^2 \\
&\leq Q\left\{\|u_{tt}\|^2_{L^2(J_{m+1};L^2)}(\Delta t_p)^3 + \|Y_{m+1}\|_0^2 + \|Y_m\|_0^2 + \|\xi_i^{m,n+1}\|_0^2\right\} \\
&\quad + \varepsilon\|\nabla\xi_i^{m,n+1}\|_0^2,
\end{aligned} \tag{11.11}$$

where the Lipschitz character of $D(U)$ [8] was used and Q depends on $\|\nabla C_i^\dagger\|_{L^\infty}$ and $\|\nabla c_i\|_{L^\infty}$. Next, by (10.3) and (10.2) with $s \geq 2$, the second term can be bounded as follows:

(11.12)

$$\begin{aligned}
&-\left(r_i^L\left(\frac{c_i^{m,n+1} - c_i^{m,n}}{\Delta t_c} - \frac{C_i^{\dagger,m,n+1} - C_i^{\dagger,m,n}}{\Delta t_c}\right), \xi_i^{m,n+1}\right) \\
&\leq Q\Bigg\{\|c_i^{m,n+1} - C_i^{\dagger,m,n+1}\|_0^2 + \left\|\frac{\partial c_i}{\partial t} - \frac{\partial C_i^\dagger}{\partial t}\right\|^2_{L^2(J_{m,n+1};L^2)}(\Delta t_c)^{-1} \\
&\quad + \|\xi_i^{m,n+1}\|_0^2\Bigg\} \\
&\leq Q\left\{\|c_i\|^2_{L^\infty(H^s)}h_c^{2s} + \|c_i\|^2_{H^1(J_{m,n+1};H^s)}(\Delta t_c)^{-1}h_c^{2s} + \|\xi_i^{m,n+1}\|_0^2\right\}.
\end{aligned}$$

The fourth term is bounded using the approximate characteristic direction

$$\tau_{I_i}(x,t) = \frac{(Iu^{m,n+1}, r_i^L)}{\sqrt{|Iu^{m,n+1}|^2 + (r_i^L)^2}} \approx \tau_i(x,t), \tag{11.13}$$

along with $c_i^{m,n+1} - \overset{\vee}{c}{}_i^{m,n+1} = c_i^{m,n+1} - \overset{\vee}{\bar{c}}{}_i^{m,n} + (1-\theta_i^{m,n})(\overset{\vee}{\bar{c}}{}_i^{m,n} - \overset{\vee}{\bar{c}}{}_i^{\#m,n})$. We have

(11.14)

$$
\begin{aligned}
&-\left(\left[r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + Iu^{m,n+1}\cdot\nabla c_i^{m,n+1}\right] - r_i^L \frac{c_i^{m,n+1} - \overset{\vee}{c}{}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right)\\
&= -\left(\sqrt{|Iu^{m,n+1}|^2 + (r_i^L)^2}\,\frac{\partial c_i^{m,n+1}}{\partial \tau_{I_i}} - r_i^L \frac{c_i^{m,n+1} - \overset{\vee}{\bar{c}}{}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right)\\
&\quad -\left(r_i^L \frac{\overset{\vee}{\bar{c}}{}_i^{m,n} - \overset{\vee}{\bar{c}}{}_i^{\#m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right)\cdot(1-\theta_i^{m,n})\\
&\le Q\left\{\left\|\frac{\partial^2 c_i}{\partial \tau_{I_i}^2}\right\|^2_{L^2(J_{m,n+1};L^2)} \Delta t_c + \|\xi_i^{m,n+1}\|_0^2 + (\Delta t_c)^3 \|u\|^2_{L^\infty(W^1_\infty)} \|c_i^{m,n}\|_1^2\right\},
\end{aligned}
$$

where the first part of the inequality is due to the backward finite difference approximation

$$
(11.15)\qquad r_i^L \frac{c_i^{m,n+1} - \bar{c}_i^{m,n+1}}{\Delta t_c} \approx \sqrt{|Iu^{m,n+1}|^2 + (r_i^L)^2}\,\frac{\partial c_i^{m,n+1}}{\partial \tau_{I_i}}
$$

and the second part comes from Lemma 11.1.

The following lemma, which was proved in [21] and [14], will be useful in dealing with a few terms.

LEMMA 11.2. *Let $f \in L^2(\Omega)$ be Ω-periodic and let $\mu, \beta \in (W^1_\infty(\Omega))^3$. For θ, $h \in \mathbf{R}$, let*

$$
(11.16)\qquad
\begin{aligned}
\overset{\vee}{f}(x) &= \theta\,\overset{\vee}{\bar{f}}(x) + (1-\theta)\,\overset{\vee}{\bar{f}}{}^{\#}(x)\\
&= \theta f(x-\mu(x)\Delta t) + (1-\theta) f(x-\beta(x)\Delta t),
\end{aligned}
$$

and assume that

$$
|\mu(x) - \beta(x)| \le Q\Delta t_c.
$$

Then,

$$
(11.17)\qquad \|\overset{\vee}{f} - f\|_{-1} \le Q\|f\|_0 \Delta t_c.
$$

Applying Lemma 11.2 to the fifth and sixth terms gives

$$\left(r_i^L \frac{(\check{c}_i^{\,m,n} - \check{C}_i^{\dagger\, m,n}) - (c_i^{m,n+1} - C_i^{\dagger,m,n})}{\Delta t_c}, \xi_i^{m,n+1} \right) \tag{11.18}$$

$$\leq Q\|c_i^{m,n} - C_i^{\dagger,m,n}\|_0^2 + \varepsilon\|\xi_i^{m,n+1}\|_1^2$$

and

$$\left(r_i^L \frac{\check{\xi}_i^{\,m,n} - \xi_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1} \right) \leq Q\|\xi_i^{m,n}\|_0^2 + \varepsilon\|\xi_i^{m,n+1}\|_1^2, \tag{11.19}$$

respectively.

In treating the seventh and eighth terms, consider generally

$$\left(r_i^L \frac{\widehat{\varphi}^{m,n} - \check{\varphi}^{\,m,n}}{\Delta t_c}, \chi \right)$$

$$= \theta_i^{m,n} \left(r_i^L \frac{\widehat{\overline{\varphi}}^{m,n} - \check{\overline{\varphi}}^{\,m,n}}{\Delta t_c}, \chi \right) \tag{11.20}$$

$$+ (1 - \theta_i^{m,n}) \left(r_i^L \frac{\widehat{\overline{\varphi}}^{\#m,n} - \check{\overline{\varphi}}^{\,\#m,n}}{\Delta t_c}, \chi \right).$$

The first term on the right-hand-side of (11.20) can be treated by following ideas which are contained in the papers mentioned above:

$$\theta_i^{m,n} \left| \left(r_i^L \frac{\widehat{\overline{\varphi}}^{m,n} - \check{\overline{\varphi}}^{\,m,n}}{\Delta t_c}, \chi \right) \right| \tag{11.21}$$

$$\leq Q \left| \left(\int_0^1 \nabla\varphi^{m,n} \left(\check{\overline{x}}^{\,m,n+1} + \frac{IY^{m,n+1}}{r_i^L} \Delta t_c s \right) \cdot IY^{m,n+1} ds, \chi \right) \right|$$

$$\leq Q\|\nabla\varphi^{m,n}\|_{L^\infty}\|IY^{m,n+1}\|_0\|\chi\|_0.$$

For the second term in (11.20), we let

$$\check{x}^{\,\#*} = x - \frac{Iu^{m,n}}{r_i^L}\Delta t_c \pm \kappa \frac{Iu^{m,n}}{r_i^L}(\Delta t_c)^2$$

and

$$\widehat{x}^{\#*} = x - \frac{IU^{m,n}}{r_i^L}\Delta t_c \pm \kappa \frac{IU^{m,n}}{r_i^L}(\Delta t_c)^2,$$

and use the ideas for the previous estimate:

$$(1-\theta_i^{m,n})\left(r_i^L\frac{\widehat{\varphi}^{\#m,n}-\overset{\vee}{\varphi}{}^{\#m,n}}{\Delta t_c},\chi\right)$$

(11.22)

$$\begin{aligned}
&=\frac{(1-\theta_i^{m,n})}{\Delta t_c}\int_\Omega\left(r_i^L\int_{\overset{\vee}{x}{}^{\#*}}^{\widehat{x}^{\#*}}\frac{\partial\varphi^{m,n}}{\partial s}ds\right)\chi\,dx\\
&=\frac{(1-\theta_i^{m,n})}{\Delta t_c}\int_\Omega r_i^L\left[\int_0^1\frac{\partial\varphi^{m,n}}{\partial s}\left((1-\overline{s})\overset{\vee}{x}{}^{\#*}+\overline{s}\widehat{x}^{\#*}\right)d\overline{s}\right]\\
&\quad\times|\overset{\vee}{x}{}^{\#*}-\widehat{x}^{\#*}|\chi\,dx\\
&\le(1-\theta_i^{m,n})(1+\kappa\Delta t_c)\times\\
&\quad\int_\Omega\left[\int_0^1\frac{\partial\varphi}{\partial s}\left((1-\overline{s})\overset{\vee}{x}{}^{\#*}+\overline{s}\widehat{x}^{\#*}\right)d\overline{s}\right]|I(u^{m,n}-U^{m,n})|\chi\,dx,
\end{aligned}$$

where s is the unit vector in the direction $\widehat{x}^{\#*}-\overset{\vee}{x}{}^{\#*}$, $\overline{s}\in[0,1]$ is a parameter for the segment connecting $\overset{\vee}{x}{}^{\#*}$ to $\widehat{x}^{\#*}$, and the estimate

$$|\widehat{x}^{\#*}-\overset{\vee}{x}{}^{\#*}|\le\frac{\Delta t_c}{r_i^L}(1+\kappa\Delta t_c)|I(u^{m,n+1}-U^{m,n+1})| \tag{11.23}$$

was used. Now letting

$$g_\varphi=\int_0^1\frac{\partial\varphi}{\partial s}\left((1-\overline{s})\overset{\vee}{x}{}^{\#*}+\overline{s}\widehat{x}^{\#*}\right)d\overline{s}, \tag{11.24}$$

we can bound (11.22) by

$$\begin{aligned}
&Q\|g_\varphi\|_{L^\infty}\|I(u^{m,n+1}-U^{m,n+1})\|_0\|\chi\|_0\\
&\le Q\|g_\varphi\|_\infty(\|Y_{m+1}\|_0+\|Y_m\|_0)\|\chi\|_0\\
&\le Q\|\nabla\varphi\|_\infty(\|Y_{m+1}\|_0+\|Y_m\|_0)\|\chi\|_0.
\end{aligned} \tag{11.25}$$

The last inequality is obtained by viewing g_φ as an average of certain first partial derivatives of φ.

Following the ideas in [15] with

$$\|U\|_{L^\infty(L^\infty)}\le Q, \tag{11.26}$$

another bound for (11.22) is

$$\begin{aligned}
&Q\|g_\varphi\|_0(\|Y_{m+1}\|_0+\|Y_m\|_0)\|\chi\|_\infty\\
&\le Q\|\nabla\varphi\|_0(\|Y_{m+1}\|_0+\|Y_m\|_0)\|\chi\|_\infty.
\end{aligned} \tag{11.27}$$

Combining (11.21) and (11.25) implies that

$$\left|\left(r_i^L \frac{\widehat{\varphi}^{m,n} - \overset{\vee}{\varphi}{}^{m,n}}{\Delta t_c}, \chi\right)\right| \leq Q\|\nabla\varphi^{m,n}\|_{L^\infty}(\|Y_{m+1}\|_0 + \|Y_m\|_0)\|\chi\|_0. \tag{11.28}$$

The following expression is another bound, which is derived by combining (11.21) and (11.27):

$$\left|\left(r_i^L \frac{\widehat{\varphi}^{m,n} - \overset{\vee}{\varphi}{}^{m,n}}{\Delta t_c}, \chi\right)\right| \leq Q\|\nabla\varphi^{m,n}\|_0(\|Y_{m+1}\|_0 + \|Y_m\|_0)\|\chi\|_\infty. \tag{11.29}$$

Douglas [6] cites a theorem of Bramble [2] which implies that, for two dimensions,

$$\|\xi^{m,n}\|_\infty \leq Q|\log\, h_c|^{\frac{1}{2}}\|\xi^{m,n}\|_1. \tag{11.30}$$

This inequality is the only place that the case of a two-dimensional domain is distinguished from that for a three-dimensional domain; the modifications required to treat three space are discussed in §12 and are essentially trivial.

Apply (11.25) to the seventh term to get

$$\begin{aligned}
&\left|-\left(r_i^L \frac{\widehat{C^\dagger}_i^{m,n} - \overset{\vee}{C^\dagger}{}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right)\right| \\
&\leq Q\|\nabla\widehat{C^\dagger}_i^{m,n}\|_\infty(\|Y_{m+1}\|_0 + \|Y_m\|_0)\|\xi_i^{m,n+1}\|_0 \\
&\leq Q(\|Y_{m+1}\|_0 + \|Y_m\|_0)\|\xi_i^{m,n+1}\|_0, \\
&\leq Q(\|Y_{m+1}\|_0^2 + \|Y_m\|_0^2) + Q\|\xi_i^{m,n+1}\|_0^2,
\end{aligned} \tag{11.31}$$

where (10.4) was used.

Next, apply (11.29) to the eighth term and use (11.30) to obtain

$$\begin{aligned}
&\left(r_i^L \frac{\widehat{\xi}_i^{m,n} - \overset{\vee}{\xi}{}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
&\leq Q\|\nabla\xi_i\|_0(\|Y_{m+1}\| + \|Y_m\|)|\log\, h_c|^{\frac{1}{2}}\|\xi_i^{m,n+1}\|_1 \\
&\leq Q(\|Y_{m+1}\| + \|Y_m\|)|\log\, h_c|^{\frac{1}{2}}\|\xi_i^{m,n+1}\|_1^2.
\end{aligned} \tag{11.32}$$

Since $(\|Y_{m+1}\| + \|Y_m\|) = o(|\log h_c|)^{-1/2}$, the above can be bounded by

$$\epsilon \|\xi_i^{m,n+1}\|_1^2. \tag{11.33}$$

Using (10.2), we can bound the ninth and tenth terms in (11.7) as follows:

$$\begin{aligned} &\left(\lambda_{i-1} r_{i-1}^L (c_{i-1}^{m,n+1} - C_{i-1}^{\dagger,m,n+1}), \xi_i^{m,n+1}\right) \\ &+ (\lambda_{i-1} r_{i-1}^L \xi_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\ &\leq Q \left\{ \|\xi_i^{m,n+1}\|_0^2 + h_c^{2s} \|c_{i-1}^{m,n+1}\|_s^2 + \|\xi_{i-1}^{m,n+1}\|_0^2 \right\}. \end{aligned} \tag{11.34}$$

The final four terms can be bounded in the following way:

$$\begin{aligned} &(q^+ E(\Delta t_c) C_i^{m,n+1}, \xi_i^{m,n+1}) - (q^+ C_i^{\dagger,m,n+1}, \xi_i^{m,n+1}) \\ &\quad + \left(\gamma_0 (c_i^{m,n+1} - C_i^{\dagger,m,n+1}), \xi_i^{m,n+1}\right) \\ &\quad + \left(\lambda_i r_i^L (E(\Delta t_c)(C_i^{m,n+1}) - c_i^{m,n+1}), \xi_i^{m,n+1}\right) \\ &= -(q^+ E(\Delta t_c)(\xi_i^{m,n+1}), \xi_i^{m,n+1}) \\ &\quad + (q^+ E(\Delta t_c)(C_i^{\dagger,m,n+1} - c_i^{m,n+1}), \xi_i^{m,n+1}) \\ &\quad + (q^+ (E(\Delta t_c)(c_i^{m,n+1}) - c_i^{m,n+1}), \xi_i^{m,n+1}) \\ &\quad + ((q^+ + \gamma_0)(c_i^{m,n+1} - C_i^{\dagger,m,n+1}), \xi_i^{m,n+1}) \\ &\quad - (\lambda_i r_i^L E(\Delta t_c)(\xi_i^{m,n+1}), \xi_i^{m,n+1}) \\ &\quad + (\lambda_i r_i^L E(\Delta t_c)(C_i^{\dagger,m,n+1} - c_i^{m,n+1}), \xi_i^{m,n+1}) \\ &\quad + (\lambda_i r_i^L E(\Delta t_c)(c_i^{m,n+1}) - c_i^{m,n+1}, \xi_i^{m.n+1}) \\ &\leq Q \Big\{ \|\xi_i^{m,n-1}\|_0^2 + \|\xi_i^{m,n}\|_0^2 + \|\xi_i^{m,n+1}\|_0^2 + h_c^{2s} \|c_i^{m,n}\|_s^2 \\ &\quad + h_c^{2s} \|c_i^{m,n-1}\|_0^2 + h_c^{2s} \|c_i^{m,n+1}\|_0^2 \\ &\quad \left\| \frac{\partial c_i}{\partial t} \right\|_{L^2(J_{m,n;L^2})}^2 (\Delta t_c) + \left\| \frac{\partial c_i}{\partial t} \right\|_{L^2(J_{m,n+1;L^2})}^2 (\Delta t_c) \Big\} \end{aligned} \tag{11.35}$$

The inequality (11.8) and the bounds obtained above for the right-hand side of (11.7) imply that

(11.36)

$$\frac{1}{2\Delta t_c}\left[(r_i^L\xi_i^{m,n+1},\xi_i^{m,n+1})-(r_i^L\xi_i^{m,n},\xi_i^{m,n})\right]+K_i\|\nabla\xi_i^{m,n+1}\|_0^2$$
$$\le Q\Big\{\|u_{tt}\|^2_{L^2(J_{m+1};L^2)}(\Delta t_p)^3+\|Y_{m+1}\|_0^2+\|Y_m\|_0^2+\|\xi_i^{m,n+1}\|_0^2+\|\xi_i^{m,n}\|_0^2$$
$$+\|\xi_i^{m,n-1}\|_0^2+\|c_i\|^2_{L^\infty(H^s)}h_c^{2s}+\|c_i\|^2_{H^1(J_{m,n+1};H^s)}(\Delta t_c)^{-1}h^{2s}$$
$$+\left(\left\|\frac{\partial^2 c_i}{\partial\tau_{I_i}^2}\right\|^2_{L^2(J_{m,n+1},L^2)}+\left\|\frac{\partial c_i}{\partial t}\right\|^2_{L^2(J_{m,n+1}\cup J_{m,n},L^2)}\right)(\Delta t_c)$$
$$+\|u\|^2_{L^\infty(W^1_\infty)}\|c_i^{m,n}\|_1^2(\Delta t_c)^3+\|c_{i-1}^{m,n+1}\|_s^2h_c^{2s}$$
$$+\|\xi_{i-1}^{m,n+1}\|_0^2\Big\}+\varepsilon\|\nabla\xi_i^{m,n+1}\|_0^2.$$

For the next step, we use Lemma 7.1, which implies that

$$\sum_{m,n}\|Y_m\|_0^2\Delta t_c\le Q\|u\|^2_{L^\infty(H^r)}h_p^{2r},\qquad 0\le r\le r^*. \tag{11.37}$$

Now, multiply (11.36) by Δt_c, sum over m and n, and absorb $\varepsilon\|\nabla\xi_i^{m,n+1}\|_0^2$ into the left-hand side to observe that

$$\sum_{m,n}\|\nabla\xi_i^{m,n+1}\|_0^2\Delta t_c+\max_{m,n}\|\xi_i^{m,n}\|_0^2 \tag{11.38}$$
$$\le Q\Big\{\sum_{m,n}\|u_{tt}\|^2_{L^2(J_{m+1};L^2)}(\Delta t_p)^3\Delta t_c+\|u\|^2_{L^\infty(H^r)}h_p^{2r}$$
$$+\sum_{m,n}\|\xi_i^{m,n+1}\|_0^2\Delta t_c+\sum_{m,n}\|c_i\|^2_{L^\infty(H^s)}h_c^{2s}\Delta t_c$$
$$+\sum_{m,n}\|c_i\|^2_{H^1(J_{m,n+1};H^s)}h_c^{2s}$$
$$+\sum_{m,n}\left(\left\|\frac{\partial^2 c_i}{\partial\tau_{I_i}^2}\right\|^2_{L^2(J_{m,n+1};L^2)}+\left\|\frac{\partial c_i}{\partial t}\right\|^2_{L^2(J_{m,n+1};L^2)}\right)(\Delta t_c)^2$$
$$+\sum_{m,n}\|u\|^2_{L^\infty(W^1_\infty)}\|c_i^{m,n}\|_1^2(\Delta t_c)^4+\sum_{m,n}\|c_{i-1}^{m,n+1}\|_s^2h_c^{2s}\Delta t_c$$
$$+\sum_{m,n}\|\xi_{i-1}^{m,n+1}\|_0^2\Delta t_c\Big\}$$

Recalling that $\Delta t_c \leq \Delta t_p$, we let

(11.39)
$$\mathcal{E}_i = \Bigg(\Big(\Big\| \frac{\partial^2 c_i}{\partial \tau_{I_i}^2} \Big\|_{L^2(L^2)} + \Big\| \frac{\partial c_i}{\partial t} \Big\|_{L^2(L^2)} \Big) \Delta t_c + \|u_{tt}\|_{L^2(L^2)} (\Delta t_p)^2 + \|u\|_{L^\infty(H^r)} h_p^r + \Big(\|c_{i-1}\|_{L^\infty(H^s)} + \|c_i\|_{L^\infty(H^s)} + \|c_i\|_{H^1(H^s)} \Big) h_c^s + \|u\|_{L^\infty(W^1_\infty)} \|c_i\|_{L^\infty(H^1)} (\Delta t_c)^{3/2} \Bigg).$$

Then, for each i,

$$\max_{m,n} \|\xi_i^{m,n}\|_0^2 + \sum_{m,n} \Big(\|\nabla \xi_i^{m,n+1}\|_0^2 \Big) \Delta t_c \leq Q \Big\{ \mathcal{E}_i^2 + \sum_{m,n} \|\xi_i^{m,n+1}\|_0^2 \Delta t_c + \sum_{m,n} \|\xi_{i-1}^{m,n+1}\|_0^2 \Delta t_c \Big\}. \tag{11.40}$$

Finally, using the discrete Gronwall inequality inductively ($\xi_0 = 0$), we see that, for $i = 1, \ldots, N$,

$$\max_{m,n} \|\xi_i^{m,n}\|_0^2 + \sum_{m,n} \|\nabla \xi_i^{m,n+1}\|_0^2 \Delta t_c \leq \sum_{i=1}^{N} \mathcal{E}_i^2, \tag{11.41}$$

and the proof is finished. □

12. Remarks

It is possible to extend these results to three space dimensions. Because we assume that the viscosity is independent of the concentration of each of the elements, the analysis does not change much. Further requirements for the extension to three dimensions are to assume that $c \in L^\infty(H^3)$, $p \in L^\infty(H^2)$, and $u \in L^\infty(H^2(div))$. These assumptions will allow the bounds $\|C^\dagger\|_{L^\infty(W^1_\infty)} \leq Q$ and $\|U\|_{L^\infty(L^\infty)} \leq Q$. Then, assuming that (11.30) could be replaced by $h_c^{-1/2}\|\xi^{m,n}\|_1$, the entire proof will still go through.

13. Derivation of equation (11.7)

We want to subtract (9.17) evaluated at time $t^{m,n+1}$ from (10.1) evaluated at time $t^{m,n+1}$, and replace χ by $\xi_i^{m,n+1}$. With these substitutions, we rewrite (10.1) and (9.17), respectively, in the following equations:

$$
\begin{aligned}
&(D_i(u^{m,n+1})\nabla C_i^{\dagger,m,n+1}, \nabla\xi_i^{m,n+1}) \\
&\quad + ((q^+ + \gamma_0)C_i^{\dagger,m,n+1}, \xi_i^{m,n+1}) \\
&\quad = -\left(r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + u^{m,n+1}\cdot\nabla c_i^{m,n+1}, \xi_i^{m,n+1}\right) \\
&\quad + (-\lambda_i r_i^L c_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L c_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (q^{+,m,n+1}\tilde{c}_i^{m,n+1}, \xi_i^{m,n+1}) + (\gamma_0 c_i, \xi_i^{m,n+1}),
\end{aligned} \tag{13.1}
$$

$$
\begin{aligned}
&\left(r_i^L \frac{C_i^{m,n+1} - \widehat{C}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
&\quad + (D_i(IU^{m,n+1})\nabla C_i^{m,n+1}, \nabla\xi_i^{m,n+1}) \\
&\quad = \left(q^{+,m,n+1}(\tilde{c}_i^{m,n+1} - E(\Delta t_c)C_i^{m,n+1}), \xi_i^{m,n+1}\right) \\
&\quad + (-\lambda_i r_i^L E(\Delta t_c)C_i^{m,n+1} \\
&\quad + \lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \xi_i^{m,n+1}).
\end{aligned} \tag{13.2}
$$

Recall that

$$\xi_i^{m,n} = C_i^{\dagger,m,n} - C_i^{m,n}.$$

Subtracting (13.2) from (13.1) gives

$$
\begin{aligned}
&(D_i(u^{m,n+1})\nabla C_i^{\dagger,m,n+1}, \nabla\xi_i^{m,n+1}) + (q^+ C_i^{\dagger,m,n+1}, \xi_i^{m,n+1}) \\
&\quad - \left(r_i^L \frac{C_i^{m,n+1} - \widehat{C}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
&\quad - (D_i(IU^{m,n+1})\nabla C_i^{m,n+1}, \nabla\xi_i^{m,n+1}) \\
&= -\left(r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + u^{m,n+1}\cdot\nabla c_i^{m,n+1}, \xi_i^{m,n+1}\right) \\
&\quad + (-\lambda_i r_i^L c_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L c_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (q^+ E(\Delta t_c)C_i^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\lambda_i r_i^L E(\Delta t_c)C_i^{m,n+1} - \lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\gamma_0(c_i^{m,n+1} - C_i^{\dagger,m,n+1}), \xi_i^{m,n+1}).
\end{aligned}
$$

Next, subtract the first two terms on the left-hand side from both sides to get

$$
\begin{aligned}
&-\left(r_i^L \frac{C_i^{m,n+1}-\widehat{C}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) - (D_i(IU^{m,n+1})\nabla C_i^{m,n+1}, \nabla\xi_i^{m,n+1}) \\
&= -(D_i(u^{m,n+1})\nabla C_i^{\dagger,m,n+1}, \nabla\xi_i^{m,n+1}) \\
&\quad - \left(r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + u^{m,n+1}\cdot\nabla c_i^{m,n+1}, \xi_i^{m,n+1}\right) \\
&\quad + (-\lambda_i r_i^L c_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L c_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (q^+(E(\Delta t_c)C_i^{m,n+1}), \xi_i^{m,n+1}) - (q^+ C_i^{\dagger,m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\lambda_i r_i^L E(\Delta t_c) C_i^{m,n+1}, \xi_i^{m,n+1}) - (\lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\gamma_0(c_i^{m,n+1} - C_i^{\dagger,m,n+1}), \xi_i^{m,n+1}).
\end{aligned}
$$

Now, add

$$(D_i(IU^{m,n+1})\nabla C_i^{\dagger,m,n+1}, \xi_i^{m,n+1})$$

and add

$$\left(r_i^L \frac{C_i^{\dagger,m,n+1}-\widehat{C}_i^{\dagger,m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right)$$

to both sides to arrive at

$$
\begin{aligned}
&\left(r_i^L \frac{\xi_i^{m,n+1}-\widehat{\xi}_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) + (D_i(IU^{m,n+1})\nabla\xi_i^{m,n+1}, \nabla\xi_i^{m,n+1}) \\
&= \left(r_i^L \frac{C_i^{\dagger,m,n+1}-\widehat{C}_i^{\dagger,m,n}}{\Delta t_c}, \xi_i^{m,n+1}\right) \\
&\quad + \left([D_i(IU^{m,n+1}) - D_i(u^{m,n+1})]\nabla C_i^{\dagger,m,n+1}, \nabla\xi_i^{m,n+1}\right) \\
&\quad - \left(r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + u^{m,n+1}\cdot\nabla c_i^{m,n+1}, \xi_i^{m,n+1}\right) \\
&\quad + (-\lambda_i r_i^L c_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L c_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (q^+(E(\Delta t_c)C_i^{m,n+1}), \xi_i^{m,n+1}) - (q^+ C_i^{\dagger,m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\lambda_i r_i^L (E(\Delta t_c) C_i^{m,n+1}), \xi_i^{m,n+1}) - (\lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\gamma_0(c_i^{m,n+1} - C_i^{\dagger,m,n+1}), \xi_i^{m,n+1}).
\end{aligned}
$$

Next, adding

$$\left(r_i^L \frac{\widehat{\xi}_i^{m,n} - \xi_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1} \right)$$

to both sides gives

$$\begin{aligned}
&\left(r_i^L \frac{\xi_i^{m,n+1} - \xi_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1} \right) + (D_i(IU^{m,n+1}) \nabla \xi_i^{m,n+1}, \nabla \xi_i^{m,n+1}) \\
&= \left(r_i^L \frac{\widehat{\xi}_i^{m,n} - \xi_i^{m,n}}{\Delta t_c}, \xi_i^{m,n+1} \right) + \left(r_i^L \frac{C_i^{\dagger,m,n+1} - \widehat{C}_i^{\dagger,m,n}}{\Delta t_c}, \xi_i^{m,n+1} \right) \\
&\quad + \left([D_i(IU^{m,n+1}) - D_i(u^{m,n+1})] \nabla C_i^{\dagger,m,n+1}, \nabla \xi_i^{m,n_1} \right) \\
&\quad - \left(r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + u^{m,n+1} \cdot \nabla c_i^{m,n+1}, \xi_i^{m,n+1} \right) \\
&\quad + (-\lambda_i r_i^L c_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L c_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (q^+ E(\Delta t_c) C_i^{m,n+1}, \xi_i^{m,n+1}) - (q^+ C_i^{\dagger,m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\lambda_i r_i^L E(\Delta t_c) C_i^{m,n+1}, \xi_i^{m,n+1}) - (\lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \xi_i^{m,n+1}) \\
&\quad + (\gamma_0 (c_i^{m,n+1} - C_i^{\dagger,m,n+1}), \xi_i^{m,n+1}).
\end{aligned}$$

The left-hand side is now finished. We deal with the right-hand side now. For visual clarity, we rewrite the first, second, and fourth terms on the right-hand side using only the functions that will be in inner products with $\xi_i^{m,n+1}$:

$$\begin{aligned}
&r_i^L \left(\frac{\widehat{\xi}_i^{m,n} - \xi_i^{m,n}}{\Delta t_c} \right) + r_i^L \left(\frac{C_i^{\dagger,m,n+1} - \widehat{C}_i^{\dagger,m,n}}{\Delta t_c} \right) \\
&\quad - \left(r_i^L \frac{\partial c_i^{m,n+1}}{\partial t} + u^{m,n+1} \cdot \nabla c_i^{m,n+1} \right)
\end{aligned}$$

$$
\begin{aligned}
= & -r_i^L\Big(\frac{c_i^{m,n+1}-c_i^{m,n}-(C_i^{\dagger,m,n+1}-C_i^{\dagger,m,n})}{\Delta t_c}\Big)\\
& -\Big((u^{m,n+1}-Iu^{m,n+1})\cdot\nabla c_i^{m,n+1}\Big)\\
& -\left(r_i^L\frac{\partial c_i^{m,n+1}}{\partial t}+Iu^{m,n+1}\cdot\nabla c_i^{m,n+1}\right)\\
& +\left(r_i^L\frac{c_i^{m,n+1}-\check{c}_i^{m,n+1}}{\Delta t_c}\right)+\left(r_i^L\frac{(\check{c}_i^{m,n}-\check{C}_i^{\dagger,m,n})-(c_i^{m,n}-C_i^{\dagger,m,n})}{\Delta t_c}\right)\\
& +r_i^L\left(\frac{\check{\xi}_i^{m,n}-\xi_i^{m,n}}{\Delta t_c}\right)-\left(r_i^L\frac{\widehat{C}_i^{\dagger,m,n}-\check{C}_i^{m,n}}{\Delta t}\right)+\left(r_i^L\frac{\widehat{\xi}_i^{m,n}-\check{\xi}_i^{m,n}}{\Delta t_c}\right).
\end{aligned}
$$

Finally, since

$$
\begin{aligned}
&\lambda_{i-1}r_{i-1}^L(c_{i-1}^{m,n+1}-C_{i-1}^{m,n+1})\\
&=\lambda_{i-1}r_{i-1}^L(c_{i-1}^{m,n+1}-C_{i-1}^{\dagger,m,n+1})+\lambda_{i-1}r_{i-1}^L\xi_{i-1}^{m,n+1},
\end{aligned}
$$

equation (11.7) is established.

14. Algorithm for the implicitly defined solution

Assume that the source term on the right-hand side of each concentration equation is treated implicitly. We can choose to treat the other terms either implicitly or explicitly. We present the mass-conservation technique (modification) when all terms are treated implicitly. The case where some terms on the right-hand side are treated explicitly requires trivial modification.

We begin by considering the original partial differential equation (5.4) with each concentration being evaluated at the new time step $t^{m,n+1}$. Integrating each equation over $(t^{m,n}, t^{m,n+1})\times\Omega$, using the relation $q = q^+ - q^-$, where $q^- = \max\{0,-q\}$, and collecting terms involving the unknowns on the left gives

$$
\begin{aligned}
(14.1)\qquad &\int_\Omega (r_i^L+\Delta t_c\lambda_i r_i^L+\Delta t_c q^-)c_i^{m,n+1}\,dx\\
&=\int_\Omega (r_i^L c_i^{m,n}+\Delta t_c\lambda_{i-1}r_{i-1}^L c_{i-1}^{m,n+1}+\Delta t_c\widetilde{c}_i^{m,n+1}q^{+,m,n+1})\,dx.
\end{aligned}
$$

Now, let

$$Q_i^{m,n} = \int_\Omega (r_i^L c_i^{m,n} + \Delta t_c \lambda_{i-1} r_{i-1}^L c_{i-1}^{m,n+1} + \Delta t_c \widetilde{c}_i^{m,n+1} q^{+,m,n+1})\, dx. \tag{14.2}$$

As stated earlier, two elliptic solves are required for each time step, and transport is not fractionally stepped. The algorithm is as follows:

For $i = 1, \dots, N$ perform the steps in order.

1. **The initial condition:** Find $C_i^0 \in M_{h_c}$ such that

$$(\nabla C_i^0, \nabla v) + (C_i^0, v) = (\nabla c_{i,init}, \nabla v) + (c_{i,init}, v), \qquad v \in M_{h_c}. \tag{14.3}$$

2. **The pressure step:** If $m = -1$ or $q_{m+1} \neq q_m$, find $(U_{m+1}, P_{m+1}) \in V_{h_p} \times W_{h_p}$ such that

$$(aU_{m+1}, v) - (\nabla \cdot v, P_{m+1}) = (\gamma, v), \qquad v \in V, \tag{14.4}$$

$$(\nabla \cdot U_{m+1}, w) = (q_{m+1}, w), \qquad w \in W. \tag{14.5}$$

(If $q_{m+1} = q_m$, just set $(U_{m+1}, P_{m+1}) = (U_m, P_m)$.)

3. **The conservation steps including transport and diffusion:**

(a) Compute

$$Q_i^{m,n} = \int_\Omega (r_i^L C_i^{m,n} + \Delta t_c \lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1} + \Delta t_c \widetilde{c}_i^{m,n+1} q^{+,m,n+1})\, dx. \tag{14.6}$$

(b) Set

$$\overline{x}_i = x - IU^{m,n+1} \Delta t_c / (r_i^L), \qquad Y_i^{m,n}(x) = C_i^{m,n}(\overline{x}_i).$$

(c) Find $\overline{C}_i^{m,n+1}$ such that

$$r_i^L \frac{\overline{C}_i^{m,n+1} - Y_i^{m,n}}{\Delta t_c} - \nabla \cdot (D_i^{m,n+1} \nabla \overline{C}_i^{m,n+1}) = (\widetilde{c}_i - \overline{C}_i^{m,n+1})\, q^{+,m,n+1} - \lambda_i r_i^L \overline{C}_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \quad x \in \Omega, \tag{14.7}$$

$$D_i^{m,n+1} \nabla \overline{C}_i^{m,n+1} \cdot n_\Omega = 0, \quad x \in \partial\Omega. \tag{14.8}$$

(d) Compute

$$\overline{Q}_i^{m,n+1} = \int_\Omega (r_i^L + \Delta t_c \lambda_i r_i^L + \Delta t_c q^-) \overline{C}_i^{m,n+1}\, dx. \tag{14.9}$$

If $\overline{Q}_i^{m,n+1} = Q_i^{m,n}$ then accept $\overline{C}_i^{m,n+1}$ as $C_i^{m,n+1}$ and proceed to the next contaminant or the next time step.

(e) If $\overline{Q}_i^{m,n} \neq Q_i^{m,n}$, let

$$\delta_i = \delta_i(x) = \kappa \frac{IU^{m,n+1}}{r_i^L}(\Delta t_c)^2, \tag{14.10}$$

$$\widehat{\overline{x}}_i^{+,m,n+1} = \widehat{\overline{x}}_i^{+,m,n+1}(x) = \overline{x}_i^{m,n+1} + \delta_i, \tag{14.11}$$

$$\widehat{\overline{x}}_i^{-,m,n+1} = \widehat{\overline{x}}_i^{-,m,n+1}(x) = \overline{x}_i^{m,n+1} - \delta_i, \tag{14.12}$$

(14.13)

$$Z_i^{m,n}(x) = \begin{cases} \max\{C_i^{m,n}(\widehat{\overline{x}}_i^{+,m,n+1}), C_i^{m,n}(\widehat{\overline{x}}_i^{-,m,n+1})\}, & \text{if } Q_i^{m,n} \geq \overline{Q}_i^{m,n+1}, \\ \min\{C_i^{m,n}(\widehat{\overline{x}}_i^{+,m,n+1}), C_i^{m,n}(\widehat{\overline{x}}_i^{-,m,n+1})\}, & \text{if } Q_i^{m,n} < \overline{Q}_i^{m,n+1}. \end{cases}$$

(f) Find $\widehat{C}_i^{m,n+1}$ such that

$$r_i^L \frac{\widehat{C}_i^{m,n+1} - Z_i^{m,n}}{\Delta t_c} - \nabla \cdot (D_i^{m,n+1} \nabla \widehat{C}_i^{m,n+1}) = (\widetilde{c} - \widehat{C}_i^{m,n+1})\, q^{+,m,n+1} - \lambda_i r_i^L \widehat{C}_i^{m,n+1} + \lambda_{i-1} r_{i-1}^L C_{i-1}^{m,n+1}, \quad x \in \Omega, \tag{14.14}$$

$$D_i^{m,n+1} \nabla \widehat{C}_i^{m,n+1} \cdot n_\Omega = 0, \quad x \in \partial\Omega, \tag{14.15}$$

and compute

$$\widehat{Q}_i^{m,n+1} = \int_\Omega (r_i^L + \Delta t_c \lambda_i r_i^L + \Delta t_c q^-)\, \widehat{C}_i^{m,n+1}\, dx. \tag{14.16}$$

(g) Find $\theta_i^{m,n+1}$ such that

$$\theta_i^{m,n+1} \overline{Q}^{m,n+1} + (1 - \theta_i^{m,n+1})\, \widehat{Q}_i^{m,n+1} = Q_i^{m,n},$$

and set

$$C_i^{m,n+1} = \theta_i^{m,n+1}\, \overline{C}^{m,n+1} + (1 - \theta_i^{m,n+1})\, \widehat{C}_i^{m,n+1}. \tag{14.17}$$

Clearly, the conservation relation (14.1) is satisfied.

The convergence proof for the implicit case is simplified in so far as equation (11.7) will contain fewer terms.

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