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Mixed and discontinuous finite volume element schemes for the optimal control of immiscible flow in porous media[☆]

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ABSTRACT

In this article we introduce a family of discretisations for the numerical approximation of optimal control problems governed by the equations of immiscible displacement in porous media. The proposed schemes are based on mixed and discontinuous finite volume element methods in combination with the optimise-then-discretise approach for the approximation of the optimal control problem, leading to nonsymmetric algebraic systems, and employing minimum regularity requirements. Estimates for the error (between a local reference solution of the infinite dimensional optimal control problem and its hybrid mixed/discontinuous approximation) measured in suitable norms are derived, showing optimal orders of convergence.

1. Introduction

Scope. We are interested in the accurate representation of the flow patterns produced by immiscible fluids within porous media. With the growing importance of the underlying physical processes in a variety of applications, the mathematical models used to describe this scenario have received a considerable attention in the past few decades. A popular example can be encountered in petroleum engineering, specifically in the standard process of oil recovery. The strategy there consists in injecting water (or other fluids having favourable density and viscosity properties) in such a way that the oil trapped in subsurface reservoirs is displaced mainly by pressure gradients. In its classical configuration, the technique of oil recovery by water injection employs two wells that contribute to maintain a high pressure and adequate flow rate in the oil field: an injection well from where the non-oleic liquid is injected, pushing the remaining oil towards a second, production well, from which oil is transported to the surface.

Regarding the simulation of these processes using mathematical models and numerical methods, there is a rich body of literature dealing with mixed finite element (FE) formulations where the filtration velocity and the pressure of each phase are solved at once (see, for instance, the classical works [1–4]). Mixed methods constructed using H(div)-conforming elements for the flux variable also allow for local mass conservation [5]. Alternative methods, also widely used in a variety of different formulations, include discontinuous Galerkin (DG) schemes which do not require inter-element continuity and feature element-wise conservation, arbitrary accuracy, controlled numerical diffusion, and can handle more adequately

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problems with rough coefficients (see, for instance, [6] for a general overview on DG methods and [7–10] for their application in different configurations of multiphase flows).

A recurrent strategy in the design of numerical methods for coupled flow-transport problems as the one described above, is to combine different techniques with the objective of retaining the main properties of each compartmental scheme. For example, combined mixed FE and DG methods have been applied in [11,12,7] to numerically solve the coupled system of miscible displacement in porous media. On the other hand, a mixed finite volume element (FVE) method approximating the velocity–pressure pair and a discontinuous finite volume element (DFVE) scheme for the saturation equation are combined in [13]. FVE schemes require the definition of trial and test spaces associated with primal and dual partitions of the domain, respectively. Different types of dual meshes are employed when the FVE method is of conforming, non-nonconforming, or discontinuous type (see details and comparisons in e.g. [14–16]), but in most cases they feature local conservativity as well as suitability for deriving L^2−error estimates. We point out that schemes belonging to the particular class of DFVE approximations preserve features of both DG and general FVE methods, including smaller support of dual elements (when compared with conforming and non-conforming FVEs) and appropriateness in handling discontinuous coefficients.

Also in the context of FVE methods, the development in [17,18] uses a mixed (or hybrid) conforming–nonconforming discretisation applied to sedimentation problems, [19,20] analyse DFVE methods applied to viscous flow and degenerate parabolic equations, and [21] introduces mixed FE in combination with DFVE for a general class of multiphase problems. An extensive survey on different methods for multiphase multicomponent flows in porous media can be found in [22–24].

Optimal control and immiscible flow in porous media. Oil recovery in its so-called primary and secondary stages, can only lead to the extraction of 20%–40% of the reservoir's original oil. Other techniques (including a tertiary stage and the enhanced oil recovery process) can increase these numbers up to 30%–60%, but the development of control devices for manipulating the progression of the oil–water front, therefore increasing further the oil recovery, is still a topic of high interest. A viable approach consists in solving optimal control problems subject to the equations of two-phase incompressible immiscible flow in porous media. The goal is quite clear: to achieve optimal oil recovery from underground reservoirs after a fixed time interval. Several variables enter into consideration (as the price of oil and water, rock porosity and intrinsic permeability, the mobilities of the fluids, the constitutive relations defining capillary pressure, and so on) but here we will restrict the study to the adjustment of the water injection only.

Control theory and adjoint-based methods have been exploited in the optimisation of several aspects of the process, for instance in the design of valve operations for wells (see e.g. [25,26] and the review paper [27]). However, and in contrast with the situation observed for the approximation of direct systems, the numerical *analysis* of optimal control problems governed by incompressible flows in porous media (meaning rigorous error estimates and stability properties) has been so far restricted to classical discretisations. These include the FE method for immiscible displacement optimal control studied in [28] and the box method for the constrained optimal control problems with partially miscible two phase flow in porous media considered in [29]. Our goal here is to investigate optimal control problems governed by two-phase incompressible immiscible flow in porous media and their discretisation using a combined mixed FVE discretisation for the flow equations, and a DFVE scheme for the approximation of the transport equation. We concentrate our development on the optimise-then-discretise approach, where one first formulates the continuous optimality conditions and then the discretisation is applied to the continuous optimal system (see its applicability in similar scenarios in e.g. [30,31]).

Outline. The remainder of the paper is organised as follows. In Section 2 we state the model problem together with the corresponding optimality conditions, and present some preliminary results. This section also contains the main assumptions required on the model coefficients. Section 3 provides details about the discrete formulation, starting with the our mixed FVE/DFVE scheme applied to the optimal control problem under consideration. We also state useful properties of the discrete operators in Lemma 3.2, and finalise the section with the specification of the time discretisation scheme. In Section 4 we advocate the derivation of a priori error estimates in suitable norms. In fact, the main results of the paper are constituted by Theorems 4.3 and 4.4, where the *a priori* error estimates of optimal order are obtained for state, costate and control variables. Appendix A contains the proof of one auxiliary result needed for the error bounds, and Appendix B gives an overview of the implementation strategy employed in the solution of the overall optimal control problem.

2. Governing equations

We consider an optimal control problem governed by a nonlinear coupled system of equations representing the interaction of two incompressible fluids in a porous structure $\Omega \subset \mathbb{R}^2$. We study the process occurring within the time interval $J = (0, T]$, where the optimisation problem reads

$$\min_{q\in Q_{\mathrm{ad}}} \mathcal{J}(q) := \frac{1}{2}\int_\Omega \tilde{w}c^2(T)\,\mathrm{d}\boldsymbol{x} + \frac{\alpha_0}{2}\int_0^T\int_\Omega \delta_0 q(t)^2\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t, \tag{2.1}$$

subject to

$$\begin{aligned} \boldsymbol{u} &= -\kappa(\boldsymbol{x})\lambda(c)\nabla p, && \forall(\boldsymbol{x},t)\in\Omega\times J,\\ \nabla\cdot\boldsymbol{u} &= (\delta_0-\delta_1)q(t), && \forall(\boldsymbol{x},t)\in\Omega\times J,\\ \phi\partial_t c - \nabla\cdot(\kappa(\boldsymbol{x})(\lambda\lambda_o\lambda_w p_c')(c)\nabla c) + \lambda_o'(c)\boldsymbol{u}\cdot\nabla c &= -\lambda_o(c)\delta_0 q(t), && \forall(\boldsymbol{x},t)\in\Omega\times J. \end{aligned} \tag{2.2}$$

Here $c(\boldsymbol{x}, t)$ represents the saturation of oil in the two-phase fluid, $\phi(\boldsymbol{x})$ the porosity of the rock, $\kappa(\boldsymbol{x})$ the permeability of the porous rock, $\lambda(c)$ the total mobility of the two-phase fluid, $\lambda_o(c)$ the relative mobility of the oil, $\lambda_w(c)$ the relative mobility of the water, $\boldsymbol{u}(\boldsymbol{x}, t)$ the Darcy velocity of the fluid mixture, $q(t)$ the flow rate of water, $p_c(c)$ the capillary pressure, $\tilde{w}$ the price of oil, α_0 the price of water. The terms δ_0 and δ_1 are Dirac functions located at the injection and production wells, respectively. For a given $\hat{q} > 0$, by $Q_{\rm ad}$ we denote the set of admissible controls

$$Q_{\rm ad} = \{q \in L^\infty[0, T] : 0 \le q \le \hat{q}\}.$$

The overall mechanism consists in finding a control q over a time interval $[0, T]$ that minimises the remaining oil in the reservoir by adjusting the amount of injected water.

For sake of the analysis and discretisation of the problem, we rewrite the system equations in a slightly different notation. Let us introduce the functions

$$\alpha(c) = [\kappa(\boldsymbol{x})\lambda(c)]^{-1}, \quad \mathcal{D}(c) = \kappa(\boldsymbol{x})\lambda(c)\lambda_o(c)\lambda_w(c)p_c'(c), \quad b(c) = \lambda_o'(c), \quad f(c) = -\lambda_o(c), \tag{2.3}$$

where $\mathcal{D}(c)$ is the diffusion coefficient representing the diffusive mobility of the fluid. We will assume that $0 < a_* \le \alpha^{-1}(c) \le a^*$, $\phi_* \le \phi(\boldsymbol{x}) \le \phi^*$ and $0 < d_* \le \mathcal{D}(c) \le d^*$, and we will also suppose that $\alpha(c)$, $b(c)$, $\mathcal{D}(c)$ and $f(c)$ are Lipschitz continuous functions of c. The requirements on these variables are physically motivated and they are reasonable in the context of the analysis of reservoir models (see e.g. [28, p. 690] or [1,2]). In particular, they contribute to have a saturation taking values between 0 and 1 (justifications are given in [32, p. 684]). Accordingly, we may restrict κ to lie in (0,1); however, the present analysis is also applicable for piecewise constant permeabilities. In turn, the Lipschitz continuity is required in the derivation of our error estimates presented in Section 4,. The assumptions above also serve to ensure existence of weak solutions to the set of governing equations. However, the actual correspondence between the assumed properties and the coefficients observed experimentally (which may exhibit discontinuities, anisotropy, and heterogeneities) remains to be explored.

The state system (2.2) is subject to slip velocities and zero-flux boundary conditions for the concentration:

$$\boldsymbol{u} \cdot \boldsymbol{n} = 0, \quad \text{and} \quad \mathcal{D}(c)\nabla c \cdot \boldsymbol{n} = 0, \quad \forall(\boldsymbol{x}, t) \in \partial\Omega \times J,$$

together with a compatibility zero-mean condition for the pressure

$$\int_\Omega p(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x} = 0, \quad \forall t \in J,$$

and a suitable initial datum for the saturation

$$c(\boldsymbol{x}, 0) = c_0(\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \Omega.$$

Let the points $\boldsymbol{x}_0$ and $\boldsymbol{x}_1$ denote the location of injection and production wells, respectively. In view of constructing numerical approximations using classical methods, the Dirac delta functions appearing as source terms in the mass conservation equation of (2.2) can be regularised as done in e.g. [28]. Let $\boldsymbol{x}_0 \in \Omega_0, \boldsymbol{x}_1 \in \Omega_1 \subset \Omega$, with $\Omega_0 \cap \Omega_1 = \emptyset$ and $|\Omega_0| = |\Omega_1| = \sigma$ with $0 < \sigma \ll 1$. We next proceed to define the functions

$$r_i = \begin{cases} 1/\sigma, & \boldsymbol{x} \in \Omega_i \\ 0, & \text{otherwise}, \end{cases} \quad i = 0, 1, \quad \text{and} \quad w(\boldsymbol{x}, t) = \begin{cases} \tilde{w}/\epsilon, & (\boldsymbol{x}, t) \in \Omega \times [T - \epsilon, T], \\ 0, & (\boldsymbol{x}, t) \in \Omega \times [0, T - \epsilon), \end{cases}$$

for a given $\epsilon > 0$. Then we can rewrite the optimal control problem (2.1)–(2.2) as follows

$$\min_{q \in Q_{\rm ad}} \mathcal{J}(q) := \frac{1}{2}\int_0^T \int_\Omega w(\boldsymbol{x}, t)c^2(\boldsymbol{x}, t)\, \mathrm{d}\boldsymbol{x}\, \mathrm{d}t + \frac{\alpha_0}{2}\int_0^T q(t)^2\, \mathrm{d}t, \tag{2.4}$$

subject to

$$\begin{aligned} \alpha(c)\boldsymbol{u} + \nabla p &= \boldsymbol{0}, && \forall(\boldsymbol{x}, t) \in \Omega \times J, \\ \nabla \cdot \boldsymbol{u} &= (r_0 - r_1)q, && \forall(\boldsymbol{x}, t) \in \Omega \times J, \\ \phi\partial_t c - \nabla \cdot (\mathcal{D}(c)\nabla c) + b(c)\boldsymbol{u} \cdot \nabla c &= f(c)r_0 q, && \forall(\boldsymbol{x}, t) \in \Omega \times J. \end{aligned} \tag{2.5}$$

We make the following assumptions on the system coefficients (see a similar treatment in e.g. [4]):

Assumption 2.1. There exists a uniform constant $M_0 > 0$ such that

$$\begin{aligned} &\left\|\alpha^{-1}(c)\right\|_{L^\infty(J;L^\infty(\Omega))} \le M_0, \ \|b(c)\|_{L^\infty(J;L^\infty(\Omega))} \le M_0, \\ &\|\mathcal{D}(c)\|_{L^\infty(J;L^\infty(\Omega))} \le M_0, \ \|f(c)\|_{L^\infty(J;L^\infty(\Omega))} \le M_0. \end{aligned}$$

Under Assumption 2.1, the optimal control problem (2.4)–(2.5) admits at least one solution (for details we refer to [28, Theorem 2.1]). However, as the state system comprises coupled nonlinear PDEs, the optimisation problem is non-convex and hence may exhibit multiple solutions. Therefore, we will assume a local optimal control (see a related strategy in [33]) of problem (2.4)–(2.5) which satisfies the first order necessary and second order sufficient optimality conditions.

Definition 2.1. A control $q \in Q_{\text{ad}}$ is said to be a local optimal solution of (2.4)–(2.5) in the sense of $L^2[0,T]$, if there is an $\epsilon > 0$ such that

$$\mathcal{J}(q) \leq \mathcal{J}(\tilde{q}) \quad \forall \tilde{q} \in Q_{\text{ad}} \quad \text{with} \quad \left\|\tilde{q} - q\right\|_{L^2[0,T]} \leq \epsilon.$$

Assumption 2.2. There exists $M_1 > 0$ such that

$$\|\boldsymbol{u}\|_{L^\infty(J;L^\infty(\Omega)^2)} \leq M_1, \; \|\nabla c\|_{L^\infty(J;L^\infty(\Omega))} \leq M_1,$$
$$\left\|\mathcal{D}'(c)\right\|_{L^\infty(J;L^\infty(\Omega))} \leq M_1, \; \left\|\alpha'(c)\right\|_{L^\infty(J;L^\infty(\Omega))} \leq M_1.$$

Assumptions 2.1 and 2.2 imply that the local solution q of (2.4)–(2.5) satisfies the classical first order optimality conditions, which can be formulated as

$$\int_0^T (f(c)r_0c^* - (r_0 - r_1)p^* + \alpha_0 q, \tilde{q} - q)\,\mathrm{d}t \geq 0, \quad \forall \tilde{q} \in Q_{\text{ad}}, \tag{2.6}$$

where, $(\boldsymbol{u}^*, p^*, c^*)$ is the costate velocity, costate pressure and costate saturation associated with q, and solving the adjoint system (see [28, Theorem 3.1]):

$$\begin{aligned} \alpha(c)\boldsymbol{u}^* + \nabla p^* + c^* b(c)\nabla c &= \mathbf{0}, \\ \nabla \cdot \boldsymbol{u}^* &= 0, \\ -\phi\partial_t c^* - \nabla\cdot(\mathcal{D}(c)\nabla c^*) - (b(c)\boldsymbol{u} - \mathcal{D}'(c)\nabla c)\cdot\nabla c^* + \alpha'(c)\boldsymbol{u}^*\cdot\boldsymbol{u} + r_1 q b(c)c^* &= wc, \end{aligned} \tag{2.7}$$

for a.e. $(\boldsymbol{x}, t) \in \Omega \times J$, associated with boundary conditions:

$$\boldsymbol{u}^* \cdot \boldsymbol{n} = 0, \qquad \mathcal{D}(c)\nabla c^* \cdot \boldsymbol{n} = 0, \qquad \forall (\boldsymbol{x}, t) \in \partial\Omega \times J,$$

and final condition $c^*(\boldsymbol{x}, T) = 0$. Finally, a common approach adopted for the optimal control of nonlinear systems of a more general nature than (2.4)–(2.5) (see e.g. [33–35]) is to assume that there exists $C_0 > 0$ such that

$$\mathcal{J}''(q)(\tilde{q}, \tilde{q}) \geq C_0\left\|\tilde{q}\right\|^2_{L^2[0,T]}, \quad \forall \tilde{q} \in Q_{\text{ad}}. \tag{2.8}$$

For our forthcoming analysis we recall the definition of the space $H(\text{div};\Omega) := \{\boldsymbol{v} \in L^2(\Omega)^2 : \nabla\cdot\boldsymbol{v} \in L^2(\Omega)\}$, equipped with the norm

$$\|\boldsymbol{v}\|^2_{\text{div},\Omega} := \|\boldsymbol{v}\|^2_{0,\Omega} + \|\nabla\cdot\boldsymbol{v}\|^2_{0,\Omega},$$

where $\|\cdot\|_{0,\Omega}$ will be employed throughout the text to denote the norm for both the spaces $L^2(\Omega)$ and for its vectorial counterpart $L^2(\Omega)^2$. Then we introduce the admissibility spaces for velocity and pressure

$$U = \{\boldsymbol{v} \in H(\text{div};\Omega) : \boldsymbol{v}\cdot\boldsymbol{n} = 0 \text{ on } \partial\Omega\}, \quad \text{and} \quad W = L^2(\Omega)/\mathbb{R},$$

respectively.

3. Finite-dimensional formulation

In this section we construct a mixed FVE–DFVE scheme tailored for the solution of the optimal control problem. First we will concentrate on the spatial discretisation, where we state an equivalence of discrete norms and recall an interpolation estimate that will serve to derive the convergence results analysed in Section 4,. We will then present the fully-discrete method.

Spatial discretisation. The velocity–pressure equations involved in the state and costate systems will be discretised via mixed FVE, whereas the saturation equation will follow a DFVE formulation. In turn, the approximation of the control variable will be carried out using a variational method (see [36]), where the control set is discretised by a projection of the discrete costate variables. Based on a first primal partition of the domain, we will require two additional dual meshes where the mixed and discontinuous FVE approximations will be defined.

Let us consider a regular, quasi-uniform partition $\{\mathcal{T}_h\}_{h>0}$ of $\bar{\Omega}$ into triangles K, of maximum diameter h. Let e be an interior edge shared by two elements K_1 and K_2 in $\mathcal{T}_h$ with outward unit normal vectors $\mathbf{n_1}$ and $\mathbf{n_2}$, respectively. For a generic scalar q, let $[\![q]\!] := q|_{\partial K_1}\mathbf{n_1} + q|_{\partial K_2}\mathbf{n_2}$ and $\langle q\rangle := \frac{1}{2}(q|_{\partial K_1} + q|_{\partial K_2})$ denote its jump and average value on e. For a generic vector $\mathbf{r}$, its jump and average across edge e is denoted respectively, by $[\![\mathbf{r}]\!] := \mathbf{r}|_{\partial\mathbf{K_1}}\cdot\mathbf{n_1} + \mathbf{r}|_{\partial\mathbf{K_2}}\cdot\mathbf{n_2}$ and $\langle\mathbf{r}\rangle := \frac{1}{2}(\mathbf{r}|_{\partial\mathbf{K_1}} + \mathbf{r}|_{\partial\mathbf{K_2}})$. For a boundary edge e with outward normal $\mathbf{n}$ we adopt the convention $\langle q\rangle = q$, $[\![q]\!] = q\mathbf{n}$, $\langle\mathbf{r}\rangle = \mathbf{r}$ and $[\![\mathbf{r}]\!] = \mathbf{r}\cdot\mathbf{n}$.

The finite dimensional trial spaces where approximate velocity and pressure will be sought are, respectively, the lowest order Raviart–Thomas space and the space of piecewise constants:

$$\begin{aligned} U_h &= \{\boldsymbol{v}_h \in U : \boldsymbol{v}_h|_K = (a + bx, c + by), \; \forall K \in \mathcal{T}_h\}, \\ W_h &= \{w_h \in W : w_h|_K \text{ is a constant}, \; \forall K \in \mathcal{T}_h\}. \end{aligned}$$

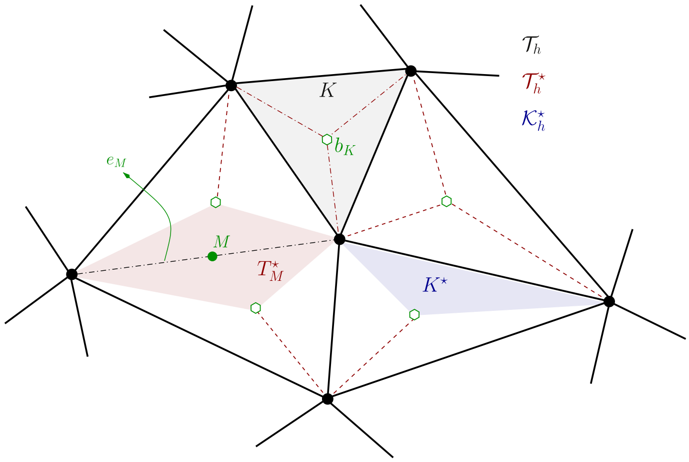

Fig. 3.1. Compound of five elements in the primal triangular mesh $\mathcal{T}_h$ (e.g. K and its barycentre b_K), and examples of one diamond element $T_M^* \in \mathcal{T}_h^*$ associated with the mid-point M of the edge e_M, and one dual element $K^* \in \mathcal{K}_h^*$.

We introduce a first dual *diamond* grid (usually employed in non-conforming FVE methods, see [14]) required for the approximation of the flow equations. The partition is denoted by $\mathcal{T}_h^*$ and its diamond elements T_M^* are quadrilaterals associated with an interior edge e_M of $\mathcal{T}_h$ (whose mid-point is M). They are formed by joining the end points of that edge to the barycentre of the triangles sharing the edge. For a boundary edge, the diamond element coincides with the boundary sub-triangle obtained by joining the end points of the boundary edge to its barycentre (see Fig. 3.1).

The test space for velocity is defined by

$$U_h^* = \{\boldsymbol{v}_h \in L^2(\Omega)^2 : \boldsymbol{v}_h|_{T_M^*} \text{ is a constant vector}, \ \forall\, T_M^* \in \mathcal{T}_h^* \text{ and } \boldsymbol{v}_h \cdot \boldsymbol{n} = 0 \text{ on } \partial\Omega\}.$$

The velocity trial and test spaces are connected by a transfer operator $\gamma_h : U_h \longrightarrow U_h^*$ defined by

$$\gamma_h \boldsymbol{v}_h(\boldsymbol{x}) = \sum_{i=1}^{N_m} \boldsymbol{v}_h(M_i)\chi_i^*(\boldsymbol{x}) \quad \forall \boldsymbol{x} \in \Omega, \tag{3.1}$$

where M_i is the mid-point of a given edge, N_m is the total number of such mid-side nodes, and χ_i^* is the characteristic function on the diamond $T_{M_i}^*$, that is,

$$\chi_i^*(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \boldsymbol{x} \in T_{M_i}^* \\ 0, & \text{otherwise.} \end{cases}$$

The following result collects some properties of γ_h, whose proof can be found in [37].

Lemma 3.1. *Let γ_h be the transfer operator defined in (3.1). Then*

$$\|\gamma_h \boldsymbol{v}_h\|_{0,\Omega} \le \|\boldsymbol{v}_h\|_{0,\Omega} \quad \forall \boldsymbol{v}_h \in U_h, \tag{3.2}$$

$$\|\boldsymbol{v}_h - \gamma_h \boldsymbol{v}_h\|_{0,\Omega} \le Ch\,\|\boldsymbol{v}_h\|_{\mathrm{div};\Omega} \quad \forall \boldsymbol{v}_h \in U_h, \tag{3.3}$$

$$b(\gamma_h \boldsymbol{v}_h, w_h) = -(\nabla \cdot \boldsymbol{v}_h, w_h) \quad \forall \boldsymbol{v}_h \in U_h,\ \forall w_h \in W_h, \tag{3.4}$$

$$(\alpha(c_h)\boldsymbol{v}_h, \gamma_h \boldsymbol{v}_h) \ge C\|\boldsymbol{v}_h\|^2_{\mathrm{div};\Omega} \quad \forall \boldsymbol{v}_h \in U_h \textit{ with } \nabla \cdot \boldsymbol{v}_h = 0. \tag{3.5}$$

For a fixed value of the approximate saturation, $\hat{c}_h$ to be made precise later, let us consider a fixed control q. Then, we can proceed as in [38] and define an approximation of the state flow equations: Find $(\hat{\boldsymbol{u}}_h, \hat{p}_h) : \bar{J} \longrightarrow U_h \times W_h$ such that for $t \in J$

$$\begin{aligned} (\alpha(\hat{c}_h)\hat{\boldsymbol{u}}_h, \gamma_h \boldsymbol{v}_h) + b(\gamma_h \boldsymbol{v}_h, \hat{p}_h) &= 0, \quad \forall \boldsymbol{v}_h \in U_h, \\ (\nabla \cdot \hat{\boldsymbol{u}}_h, w_h) - ((r_0 - r_1)q, w_h) &= 0, \quad \forall w_h \in W_h, \end{aligned}$$

where

$$b(\gamma_h \boldsymbol{v}_h, w_h) := -\sum_{i=1}^{N_m} \boldsymbol{v}_h(M_i) \cdot \int_{\partial T_{M_i}^*} w_h \boldsymbol{n}_{T_{M_i}^*}\, \mathrm{d}s \quad \forall \boldsymbol{v}_h \in U_h, \quad \forall w_h \in W_h.$$

In addition to the diamond mesh $\mathcal{T}_h^*$ we introduce a second auxiliary partition $\mathcal{K}_h^*$, on which the DFVE approximation of the saturation will be carried out. The elements in $\mathcal{K}_h^*$ are constructed by dividing each primal element $K \in \mathcal{T}_h$ into three sub-triangles by joining the barycentre b_K with the vertices of K. We can then define the trial space M_h on $\mathcal{T}_h$ and the test space L_h on $\mathcal{K}_h^*$ for the saturation approximation as

$$M_h = \{z_h \in L^2(\Omega) : z_h|_K \in \mathcal{P}_1(K) \quad \forall K \in \mathcal{T}_h\},$$
$$L_h = \{z_h \in L^2(\Omega) : z_h|_K^* \in \mathcal{P}_0(K^*) \quad \forall K^* \in \mathcal{K}_h^*\},$$

where $\mathcal{P}_k(K)$ denotes the local space of polynomials of degree up to k. We also introduce a discrete space with higher regularity $M(h) = M_h \cap H^2(\Omega)$, and (as done for the velocity approximation) we are able to map trial and test spaces thanks to the transfer operator $\eta_h : M(h) \to L_h$ defined by

$$\eta_h z|_{K^*} = \frac{1}{h_e}\int_e z|_{K^*}\,\mathrm{d}s, \qquad K^* \in \mathcal{K}_h^*, \tag{3.6}$$

with h_e denoting the length of the edge $e \in \partial K$ which is part of the dual element K^* (see Fig. 3.1). In analogy to Lemma 3.1, we now state some properties of this map, necessary in our subsequent analysis. For a proof we refer to [39,38,40].

Lemma 3.2. *For the operator η_h defined in (3.6), the following properties hold:*

1. *The norm defined by $|||z_h|||_{\eta_h}^2 := (z_h, \eta_h z_h)$, for $z_h \in M_h$, is equivalent to the L^2—norm.*
2. *The operator η_h is stable with respect to the L^2—norm. In particular*

$$\|\eta_h z_h\|_{0,\Omega} = \|z_h\|_{0,\Omega}\,, \quad \forall z_h \in M_h. \tag{3.7}$$

3. *There holds $\|z - \eta_h z\|_{0,K} \le Ch_K\,\|z\|_{1,K}$ for all $z \in M(h)$ and $K \in \mathcal{T}_h$.*

The DFVE formulation for the saturation equation in the state system for a given control q can be defined as: Find $\hat{c}_h(t) \in M_h$, $t \in \bar{J}$ such that

$$(\phi\partial_t\hat{c}_h, \eta_h z_h) + A_h(\hat{c}_h; \hat{c}_h, z_h) + (b(\hat{c}_h)\hat{\boldsymbol{u}}_h \cdot \nabla\hat{c}_h, \eta_h z_h) = (f(\hat{c}_h)r_0 q, \eta_h z_h), \quad \forall z_h \in M_h,$$

associated with initial condition $\hat{c}_h(0) = c_{0,h}$, where $\hat{c}_{0,h}$ is a Riesz projection of $c_0(\boldsymbol{x})$, and for $z, \phi, \psi \in M(h)$, the trilinear form $A_h(\cdot;\cdot,\cdot)$ is defined by

$$\begin{aligned} A_h(\psi;\phi,z) = &-\sum_{K\in\mathcal{T}_h}\sum_{j=1}^{3}\int_{v_K^{j+1}b_K v_K^j} \mathcal{D}(\psi)\nabla\phi\cdot\boldsymbol{n}\eta_h z\,\mathrm{d}s - \sum_{e\in\mathcal{E}_h}\int_e [\![\eta_h z]\!]\cdot\langle\mathcal{D}(\psi)\nabla\phi\rangle\,\mathrm{d}s \\ &- \sum_{e\in\mathcal{E}_h}\int_e [\![\eta_h\phi]\!]\cdot\langle\mathcal{D}(\psi)\nabla z\rangle\,\mathrm{d}s + \sum_{e\in\mathcal{E}_h}\int_e \frac{\xi}{h_e}[\![\phi]\!][\![z]\!]\,\mathrm{d}s, \end{aligned} \tag{3.8}$$

where v_K^j denotes a given vertex of the primal element $K \in \mathcal{T}_h$ and we adopt the convention $v_K^4 = v_K^1$. The parameter ξ is a penalisation constant, chosen independently of h. It turns out that the bilinear form defined in (3.8) is bounded and coercive with respect to the mesh dependent norm $|||\cdot|||_h$ defined by (see [41, Lemmas 2.3,2.4]):

$$|||z_h|||_h^2 := \sum_{K\in\mathcal{T}_h}|z_h|_{1,K}^2 + \sum_{e\in\mathcal{E}_h}\frac{1}{h_e}\int_e [\![z_h]\!]^2\,\mathrm{d}s.$$

Applying the combined mixed FVE/DFVE schemes for the space discretisation of the optimal control problem (2.4)–(2.5) and relation (3.4), we obtain the following semidiscrete formulation: Find $(\boldsymbol{u}_h(t), p_h(t), c_h(t), \boldsymbol{u}_h^*(t), p_h^*(t), c_h^*(t), q_h) \in U_h \times W_h \times M_h \times U_h \times W_h \times M_h \times Q_{\mathrm{ad}}$ with $t \in \bar{J}$ satisfying

$$(\alpha(c_h)\boldsymbol{u}_h, \gamma_h\boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h, p_h) = 0, \quad \forall\boldsymbol{v}_h \in U_h, \tag{3.9}$$
$$(\nabla\cdot\boldsymbol{u}_h, w_h) = ((r_0 - r_1)q_h, w_h), \quad \forall w_h \in W_h, \tag{3.10}$$
$$(\phi\partial_t c_h, \eta_h z_h) + A_h(c_h; c_h, z_h) + (b(c_h)\boldsymbol{u}_h\cdot\nabla c_h, \eta_h z_h) = (f(c_h)r_0 q_h, \eta_h z_h), \;\; \forall z_h \in M_h, \tag{3.11}$$
$$(\alpha(c_h)\boldsymbol{u}_h^*, \gamma_h\boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h, p_h^*) + (c_h^* b(c_h)\nabla c_h, \gamma_h\boldsymbol{v}_h) = 0, \quad \forall\boldsymbol{v}_h \in U_h, \tag{3.12}$$
$$(\nabla\cdot\boldsymbol{u}_h^*, w_h) = 0, \quad \forall w_h \in W_h, \tag{3.13}$$
$$\left.\begin{aligned} &-(\phi\partial_t c_h^*, \eta_h z_h) + A_h(c_h; c_h^*, z_h) - (b(c_h)\boldsymbol{u}_h\cdot\nabla c_h^*, \eta_h z_h) + (\mathcal{D}'(c_h)\nabla c_h\cdot\nabla c_h^*, \eta_h z_h) \\ &\qquad +(\alpha'(c_h)\boldsymbol{u}_h^*\cdot\boldsymbol{u}_h, \eta_h z_h) + (r_1 q_h b(c_h)c_h^*, \eta_h z_h) = (w c_h, \eta_h z_h), \;\; \forall z_h \in M_h, \end{aligned}\right\} \tag{3.14}$$
$$\int_0^T (f(c_h)r_0 c_h^* - (r_0 - r_1)p_h^* + \alpha_0 q_h, \tilde{q} - q_h)\,\mathrm{d}t \ge 0, \quad \forall\tilde{q} \in Q_{\mathrm{ad}}, \tag{3.15}$$

subject to the initial and final conditions $c_h(0) = c_{0,h}$, $c_h^*(T) = 0$.

Temporal discretisation. Let $\{t^i\}_{i=0}^N$ be a uniform partition of time interval $[0, T]$ with time step $\Delta t > 0$. We apply a backward Euler method to advance in time the optimal control system (3.9)–(3.15), leading to the following fully-discrete formulation: Find $(\boldsymbol{u}_h^i, p_h^i, c_h^{i+1}, \boldsymbol{u}_h^{*i}, p_h^{*i}, c_h^{*(i+1)}, q_h^i) \in U_h \times W_h \times M_h \times U_h \times W_h \times M_h \times Q_{\rm ad}$ such that

$$
\begin{aligned}
&(\alpha(c_h^i)\boldsymbol{u}_h^i, \gamma_h \boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h, p_h^i) = 0, \ \ i = 0, \dots, N;\\
&(\nabla\cdot\boldsymbol{u}_h^i, w_h) = ((r_0 - r_1)q_h^i, w_h), \ \ i = 0, \dots, N;\\
&(\phi \frac{c_h^{i+1} - c_h^i}{\Delta t}, \eta_h z_h) + A_h(c_h^{i+1}; c_h^{i+1}, z_h) + (b(c_h^{i+1})\boldsymbol{u}_h^i \cdot \nabla c_h^{i+1}, \eta_h z_h)\\
&\quad = (f(c_h^{i+1})r_0 q_h^{i+1}, \eta_h z_h), \ \ i = 0, \dots, N-1;\\
&(\alpha(c_h^i)\boldsymbol{u}_h^{*i}, \gamma_h \boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h, p_h^{*i}) + (c_h^{*i} b(c_h^i)\nabla c_h^i, \gamma_h\boldsymbol{v}_h) = 0, \ \ i = N, \dots, 0;\\
&(\nabla\cdot\boldsymbol{u}_h^{*i}, w_h) = 0, \ \ i = N, \dots, 0;\\
&-(\phi \frac{c_h^{*(i+1)} - c_h^{*i}}{\Delta t}, \eta_h z_h) + A_h(c_h^{i+1}; c_h^{*(i+1)}, z_h) - (b(c_h^{i+1})\boldsymbol{u}_h^i \cdot \nabla c_h^{*(i+1)}, \eta_h z_h)\\
&\quad + (\mathcal{D}'(c_h^{i+1})\nabla c_h^{i+1}\cdot\nabla c_h^{*(i+1)}, \eta_h z_h) + (\alpha'(c_h^{i+1})\boldsymbol{u}_h^{*i}\cdot\boldsymbol{u}_h^i, \eta_h z_h)\\
&\quad + (r_1 q_h^{i+1} b(c_h^{i+1})c_h^{*(i+1)}, \eta_h z_h) - (w c_h^{i+1}, \eta_h z_h) = 0, \ \ i = N-1, \dots, 0;\\
&(f(c_h^i)r_0 c_h^{*i} - (r_0 - r_1)p_h^{*i} + \alpha_0 q_h^i, \tilde{q}_h - q_h^i) \geq 0, \quad \forall \tilde{q}_h \in Q_{\rm ad}, \ i = 0, \dots, N;
\end{aligned}
$$

for all $\boldsymbol{v}_h \in U_h$, $w_h \in W_h$ and $z_h \in M_h$, with initial and terminal conditions $c_h^0 = c_{0,h}$, $c_h^{*T} = 0$.

4. Error estimates

In this section we derive suitable error bounds for the mixed FVE and DFVE approximations of (2.4)–(2.5) for a fixed local reference control satisfying the optimality conditions (2.6) and (2.8). The main results of the section will be stated below, in Theorems 4.3 and 4.4. Our theoretical analysis requires similar assumptions as those adopted in [28, Assumption (C)]. More precisely, we suppose that there exists $M_2 > 0$ such that:

$$
\begin{aligned}
&\|\alpha''(c)\|_{L^\infty(J;L^\infty)} + \|b''(c)\|_{L^\infty(J;L^\infty)} + \|\mathcal{D}''(c)\|_{L^\infty(J;L^\infty)} + \|\boldsymbol{u}\|_{L^\infty(J;L^2(\Omega)^2)} + \|\partial_t\boldsymbol{u}\|_{L^\infty(J;L^2(\Omega)^2)}\\
&\quad + \|p\|_{L^\infty(J;H^1(\Omega))}\, \|c\|_{L^\infty(J;H^2(\Omega))} + \|\partial_t c\|_{L^\infty(J;H^2(\Omega))} + \|\boldsymbol{u}^*\|_{L^\infty(J;L^2(\Omega)^2)} + \|\partial_t\boldsymbol{u}^*\|_{L^\infty(J;L^2(\Omega)^2)}\\
&\quad + \|p^*\|_{L^\infty(J;H^1(\Omega))}\, \|c^*\|_{L^\infty(J;H^2(\Omega))} + \|\partial_t c^*\|_{L^\infty(J;H^2(\Omega))} \leq M_2.
\end{aligned}
$$

These assumptions involve higher regularity of the weak solutions and are employed when invoking interpolation properties. At each time interval $[t^m, t^{m+1}]$, $m = 1, \dots, N-1$ and for a given arbitrary q^m, let the functions $(\hat{\boldsymbol{u}}_h^m, \hat{p}_h^m, \hat{c}_h^{m+1}, \hat{\boldsymbol{u}}_h^{*m}, \hat{p}_h^{*m}, \hat{c}_h^{*(m+1)})$ satisfy the following system

$$
\left.\begin{aligned}
(\alpha(\hat{c}_h^m)\hat{\boldsymbol{u}}_h^m, \gamma_h\boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h, \hat{p}_h^m) = 0, \quad \forall \boldsymbol{v}_h \in U_h,\\
(\nabla\cdot\hat{\boldsymbol{u}}_h^m, w_h) - ((r_0 - r_1)q^m, w_h) = 0, \quad \forall w_h \in W_h,
\end{aligned}\right\} \tag{4.1}
$$

$$
\left.\begin{aligned}
(\phi\frac{\hat{c}_h^{m+1} - \hat{c}_h^m}{\Delta t}, \eta_h z_h) + A_h(\hat{c}_h^{m+1}; \hat{c}_h^{m+1}, z_h) + (b(\hat{c}_h^{m+1})\hat{\boldsymbol{u}}_h^m\cdot\nabla\hat{c}_h^{m+1}, \eta_h z_h)\\
= (f(\hat{c}_h^{m+1})r_0 q^{m+1}, \eta_h z_h), \quad \forall z_h \in M_h,
\end{aligned}\right\} \tag{4.2}
$$

$$
\left.\begin{aligned}
(\alpha(\hat{c}_h^m)\hat{\boldsymbol{u}}_h^{*m}, \gamma_h\boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h, \hat{p}_h^{*m}) + (\hat{c}_h^{*m} b(\hat{c}_h^m)\nabla\hat{c}_h^m, \gamma_h\boldsymbol{v}_h) = 0, \quad \forall\boldsymbol{v}_h \in U_h,\\
(\nabla\cdot\hat{\boldsymbol{u}}_h^{*m}, w_h) = 0, \quad \forall w_h \in W_h,
\end{aligned}\right\} \tag{4.3}
$$

$$
\left.\begin{aligned}
-(\phi\frac{\hat{c}_h^{*(m+1)} - \hat{c}_h^{*m}}{\Delta t}, \eta_h z_h) + A_h(\hat{c}_h^{m+1}; \hat{c}_h^{*(m+1)}, z_h) - (b(\hat{c}_h^{m+1})\hat{\boldsymbol{u}}_h^m\cdot\nabla\hat{c}_h^{*(m+1)}, \eta_h z_h)\\
+(\mathcal{D}'(\hat{c}_h^{m+1})\nabla\hat{c}_h^{m+1}\cdot\nabla\hat{c}_h^{*(m+1)}, \eta_h z_h) + (\alpha'(\hat{c}_h^{m+1})\hat{\boldsymbol{u}}_h^{*m}\cdot\hat{\boldsymbol{u}}_h^m, \eta_h z_h)\\
+(r_1 b(\hat{c}_h^{m+1})q^{m+1}\hat{c}_h^{*(m+1)}, \eta_h z_h) = (w\hat{c}_h^{m+1}, \eta_h z_h), \quad \forall z_h \in M_h,
\end{aligned}\right\} \tag{4.4}
$$

associated with initial and terminal conditions $\hat{c}_h(0) = c_{0,h}$, $\hat{c}_h^*(T) = 0$.

The following theorem (whose proof can be found in [13]) gives an error estimate for the state variables in (4.1)–(4.4).

Theorem 4.1. *At $t = t^m$, $1 \leq m \leq N$ and for a given q^m, let $(\boldsymbol{u}^m, p^m, c^m)$ be the exact solutions and $(\hat{\boldsymbol{u}}_h^m, \hat{p}_h^m, \hat{c}_h^m)$ be the solutions of (4.1)– (4.2). Then*

$$
\|\boldsymbol{u}^m - \hat{\boldsymbol{u}}_h^m\|_{0,\Omega} + \|p^m - \hat{p}_h^m\|_{0,\Omega} + \|c^m - \hat{c}_h^m\|_{0,\Omega} \leq C(h + \Delta t).
$$

Likewise, one can derive a similar error bound for the costate variables involved in (4.1)–(4.4). The proof of this auxiliary result will be postponed to Appendix A.

Theorem 4.2. *At $t = t^m$, $1 \le m \le N$ and for a given q^m, let $(\boldsymbol{u}^{*m}, p^{*m}, c^{*m})$ be the exact solutions and $(\hat{\boldsymbol{u}}_h^{*m}, \hat{p}_h^{*m}, \hat{c}_h^{*m})$ be the solutions of (4.3)– (4.4). Then*

$$\left\|\boldsymbol{u}^{*m} - \hat{\boldsymbol{u}}_h^{*m}\right\|_{0,\Omega} + \left\|p^{*m} - \hat{p}_h^{*m}\right\|_{0,\Omega} + \left\|c^{*m} - \hat{c}_h^{*m}\right\|_{0,\Omega} \le C(h + \Delta t).$$

In what follows, for a given time t^m we will adopt the notation

$$(\boldsymbol{u}^m(q_h), p^m(q_h), c^m(q_h), \boldsymbol{u}^{*m}(q_h), p^{*m}(q_h), c^{*m}(q_h)),$$

to indicate functions satisfying the continuous optimal system for a given control q_h. This next result states the convergence of state and costate approximate flow rate of water, velocity, pressure, and concentration.

Theorem 4.3. *For a fixed $t = t^m$, $1 \le m \le N$, let q^m be a local optimal control of (2.4)– (2.5) having state and costate solutions $(\boldsymbol{u}^m, p^m, c^m, \boldsymbol{u}^{*m}, p^{*m}, c^{*m})$, and let $(q_h^m, \boldsymbol{u}_h^m, p_h^m, c_h^m, \boldsymbol{u}_h^{*m}, p_h^{*m}, c_h^{*m})$ be its discrete counterpart. Then, there exists $C > 0$ independent of h, Δt, such that:*

$$\begin{aligned}
\left\|q^m - q_h^m\right\|_{L^2(0,T)} &\le C(h + \Delta t),\\
\left\|\boldsymbol{u}^m - \boldsymbol{u}_h^m\right\|_{0,\Omega} + \left\|p^m - p_h^m\right\|_{0,\Omega} + \left\|c^m - c_h^m\right\|_{0,\Omega} &\le C(h + \Delta t),\\
\left\|\boldsymbol{u}^{*m} - \boldsymbol{u}_h^{*m}\right\|_{0,\Omega} + \left\|p^{*m} - p_h^{*m}\right\|_{0,\Omega} + \left\|c^{*m} - c_h^{*m}\right\|_{0,\Omega} &\le C(h + \Delta t).
\end{aligned}$$

Proof. The continuous and discrete variational inequalities readily imply that

$$\begin{aligned}
&(f(c^m)r_0c^{*m} - (r_0 - r_1)p^{*m} + \alpha_0 q^m, q^m - q_h^m)\\
&\qquad \le 0 \le (f(c_h^m)r_0c_h^{*m} - (r_0 - r_1)p_h^{*m} + \alpha_0 q_h^m, q^m - q_h^m).
\end{aligned} \tag{4.5}$$

On the other hand, taking $\tilde{q} = q^m - q_h^m$, and using the convexity assumption (2.8), leads to

$$\begin{aligned}
C_0\left\|q^m - q_h^m\right\|^2_{L^2(0,T)} &\le (J'(q^m) - J'(q_h^m), q^m - q_h^m),\\
&\le (f(c^{m+1})r_0c^{*m} - (r_0 - r_1)p^{*m} + \alpha_0 q^m, q^m - q_h^m)\\
&\quad - (f(c^m(q_h))r_0c^{*m}(q_h) - (r_0 - r_1)p^{*m}(q_h) + \alpha_0 q_h^m, q^m - q_h^m),
\end{aligned}$$

and from (4.5), we have

$$\begin{aligned}
C_0\left\|q^m - q_h^m\right\|^2_{L^2(0,T)} \le\ & (f(c_h^m)r_0c_h^{*m} - (r_0 - r_1)p_h^{*m} + \alpha_0 q_h^m, q^m - q_h^m)\\
&- (f(c^m(q_h))r_0c^{*m}(q_h) - (r_0 - r_1)p^{*m}(q_h) + \alpha_0 q_h^m, q^m - q_h^m)\\
=\ & (r_0(f(c_h^m)c_h^{*m} - f(c^m(q_h))c^{*m}(q_h)), q^m - q_h^m)\\
&- ((r_0 - r_1)(p_h^{*m} - p^{*m}(q_h), q^m - q_h^m)),
\end{aligned}$$

which in turn yields

$$\left\|q^m - q_h^m\right\|_{L^2(0,T)} \le C\left(\left\|c^m(q_h) - c_h^m\right\|_{0,\Omega} + \left\|c^{*m}(q_h) - c_h^{*m}\right\|_{0,\Omega} + \left\|p^{*m}(q_h) - p_h^{*m}\right\|_{0,\Omega}\right). \tag{4.6}$$

From these results, and proceeding very much in the same way as done in the proofs of Theorems 4.1 and 4.2, we can assert that

$$\left\|c^m(q_h) - c_h^m\right\|_{0,\Omega} + \left\|\boldsymbol{u}^m(q_h) - \boldsymbol{u}_h^m\right\|_{0,\Omega} + \left\|p^m(q_h) - p_h^m\right\|_{0,\Omega} \le C(h + \Delta t), \tag{4.7}$$

$$\left\|c^{*m}(q_h) - c_h^{*m}\right\|_{0,\Omega} + \left\|\boldsymbol{u}^{*m}(q_h) - \boldsymbol{u}_h^{*m}\right\|_{0,\Omega} + \left\|p^{*m}(q_h) - p_h^{*m}\right\|_{0,\Omega} \le C(h + \Delta t), \tag{4.8}$$

$$\left\|c^m - c_h^m\right\|_{0,\Omega} + \left\|\boldsymbol{u}^m - \boldsymbol{u}_h^m\right\|_{0,\Omega} + \left\|p^m - p_h^m\right\|_{0,\Omega} \le C[(h + \Delta t) + \left\|q^m - q_h^m\right\|_{L^2(0,T)}], \tag{4.9}$$

$$\left\|c^{*m} - c_h^{*m}\right\|_{0,\Omega} + \left\|\boldsymbol{u}^{*m} - \boldsymbol{u}_h^{*m}\right\|_{0,\Omega} + \left\|p^{*m} - p_h^{*m}\right\|_{0,\Omega} \le C[(h + \Delta t) + \left\|q^m - q_h^m\right\|_{L^2(0,T)}], \tag{4.10}$$

and hence the desired result follows directly from (4.6) and (4.7)–(4.10). □

Next we devote ourselves to the derivation of error estimates for the saturation in the broken H^1-norm. Let us start by introducing the trilinear form $\tilde{A}_h(\cdot;\cdot,\cdot) : M(h)^3 \to \mathbb{R}$ defined as

$$\begin{aligned}
\tilde{A}_h(\psi;\phi,z) = &-\sum_{K\in\mathcal{T}_h}\int_K \mathcal{D}(\psi)\nabla\phi\cdot\nabla z\,\mathrm{d}s - \sum_{e\in\mathcal{E}_h}\int_e [\![z]\!]\cdot\langle\mathcal{D}(\psi)\nabla\phi\rangle\,\mathrm{d}s\\
&-\sum_{e\in\mathcal{E}_h}\int_e [\![\phi]\!]\cdot\langle\mathcal{D}(\psi)\nabla z\rangle\,\mathrm{d}s + \sum_{e\in\mathcal{E}_h}\int_e \frac{\xi}{h_e}[\![\phi]\!][\![z]\!]\,\mathrm{d}s.
\end{aligned}$$

If we now fix ψ and set $\epsilon_a(\psi,\phi,\chi) := \tilde{A}_h(\psi;\phi,\chi) - A_h(\psi;\phi,\chi) \quad \forall\psi,\chi \in M_h$, then we have the following bound (see [42, Lemma 3.2])

$$\epsilon_a(\psi,\phi,\chi) \le Ch|||\phi|||_h|||\chi|||_h. \tag{4.11}$$

We are now ready to prove the convergence of state and costate approximate saturation.

Theorem 4.4. *At $t = t^m$, $1 \le m \le N$, let c^m and c^{*m} be the state and costate saturations associated with the continuous problem (2.4)– (2.5), and having discrete counterparts c_h^m and c_h^{*m}, respectively. Then, there exists $C > 0$ independent of h and Δt, such that:*

$$\left|\left|\left|c^m - c_h^m\right|\right|\right|_h + \left|\left|\left|c^{*m} - c_h^{*m}\right|\right|\right|_h \le C(h+\Delta t). \tag{4.12}$$

Proof. Let $\tilde{c}_h^n$ be the Riesz projection of c^n at time $t = t^n$ such that

$$A_h(c^n; c^n - \tilde{c}_h^n, z_h) + (b(c^n)\boldsymbol{u}^n \cdot \nabla(c^n - \tilde{c}_h^n), z_h) + \lambda(c^n - \tilde{c}_h^n, z_h) = 0, \quad \forall z_h \in M_h, \tag{4.13}$$

where $\lambda > 0$ is chosen to guarantee the coercivity of bilinear form defined by (4.13) with respect to the norm $|||\cdot|||_h$. We then proceed similarly as in [13, Lemma 4.2] and split $c^n - c_h^n = (c^n - \tilde{c}_h^n) + (\tilde{c}_h^n - c_h^n) = \rho^n + \theta^n$, which implies that

$$\left|\left|\left|c^n - c_h^n\right|\right|\right|_h \le \left|\left|\left|\rho^n\right|\right|\right|_h + \left|\left|\left|\theta^n\right|\right|\right|_h \le Ch + \left|\left|\left|\theta^n\right|\right|\right|_h. \tag{4.14}$$

Testing the state saturation equation in (2.5) against $\eta_h z_h$ and integrating over Ω, we obtain, at $t = t^{n+1}$

$$\begin{aligned}(\phi\partial_t c^{n+1}, \eta_h z_h) + A_h(c^{n+1}; c^{n+1}, z_h) + (b(c^{n+1})\boldsymbol{u}^{n+1} \cdot \nabla c^{n+1}, \eta_h z_h)\\ = (f(c^{n+1})r_0 q^{n+1}, \eta_h z_h).\end{aligned} \tag{4.15}$$

Subtracting the discrete state saturation equation from (4.15), we then obtain

$$\begin{aligned}&(\phi\partial_t\theta^{n+1}, \eta_h z_h) + A_h(c^{n+1}; c^{n+1}, z_h) - A_h(c_h^{n+1}; c_h^{n+1}, z_h) + (b(c^{n+1})\boldsymbol{u}^{n+1} \cdot \nabla c^{n+1}, \eta_h z_h)\\ &- (b(c_h^{n+1})\boldsymbol{u}_h^n \cdot \nabla c_h^{n+1}, \eta_h z_h) = -(\phi\frac{\rho^{n+1}-\rho^n}{\Delta t}, \eta_h z_h) - \phi(\partial_t c^{n+1} - \frac{c^{n+1}-c^n}{\Delta t}, \eta_h z_h)\\ &+ (f(c^{n+1})r_0 q^{n+1} - f(c_h^{n+1})r_0 q_h^{n+1}, \eta_h z_h).\end{aligned}$$

Using the definition of ϵ_a together with relation (4.13), and choosing $z_h = \partial_t\theta^{n+1}$, we arrive at

$$\begin{aligned}&\phi\left|\left|\left|\partial_t\theta^{n+1}\right|\right|\right|_{\eta_h}^2 + A(c_h^{n+1}; \theta^{n+1}, \partial_t\theta^{n+1})\\ &= -(\phi\frac{\rho^{n+1}-\rho^n}{\Delta t}, \eta_h\partial_t\theta^{n+1}) - \phi(\partial_t c^{n+1} - \frac{c^{n+1}-c^n}{\Delta t}, \eta_h\partial_t\theta^{n+1})\\ &\quad + (f(c^{n+1})r_0 q^{n+1} - f(c_h^{n+1})r_0 q_h^{n+1}, \eta_h\partial_t\theta^{n+1}) + (\lambda\rho^{n+1}, \eta_h\partial_t\theta^{n+1})\\ &\quad + [A_h(c_h^{n+1}; \tilde{c}_h^{n+1}, \partial_t\theta^{n+1}) - A_h(c^{n+1}; \tilde{c}_h^{n+1}, \partial_t\theta^{n+1})]\\ &\quad - (b(c_h^{n+1})\boldsymbol{u}_h^n \cdot \nabla c_h^{n+1}, \partial_t\theta^{n+1} - \eta_h\partial_t\theta^{n+1}) + (b(c^{n+1})\boldsymbol{u}^{n+1} \cdot \nabla c^{n+1}, \partial_t\theta^{n+1} - \eta_h\partial_t\theta^{n+1})\\ &\quad - ((b(c^{n+1})\boldsymbol{u}^{n+1} - b(c_h^{n+1})\boldsymbol{u}_h^n) \cdot \nabla\tilde{c}_h^{n+1}, \partial_t\theta^{n+1})\\ &\quad - (b(c^{n+1})\boldsymbol{u}^{n+1} \cdot \nabla\theta^{n+1}, \eta_h\partial_t\theta^{n+1}) + \epsilon_a(c_h^{n+1}; \theta^{n+1}, \partial_t\theta^{n+1}).\end{aligned} \tag{4.16}$$

We can then apply (4.11) and the inverse inequality to obtain

$$\epsilon_a(c_h^{n+1}; \theta^{n+1}, \partial_t\theta^{n+1}) \le Ch\left|\left|\left|\theta^{n+1}\right|\right|\right|_h\left|\left|\left|\partial_t\theta^{n+1}\right|\right|\right|_h \le C\left|\left|\left|\theta^{n+1}\right|\right|\right|_h \left\|\partial_t\theta^{n+1}\right\|_{0,\Omega}. \tag{4.17}$$

Proceeding similarly as in the proof of Theorem 4.2, and using (4.17), we deduce that the terms in (4.16) can be bounded as follows

$$\begin{aligned}&\phi\left|\left|\left|\partial_t\theta^{n+1}\right|\right|\right|_{\eta_h}^2 + A(c_h^{n+1}; \theta^{n+1}, \partial_t\theta^{n+1})\\ &\le C[\left\|c^{n+1} - c_h^{n+1}\right\|_{0,\Omega}^2 + \left\|\boldsymbol{u}^n - \boldsymbol{u}_h^n\right\|_{0,\Omega}^2 + \left\|q^{n+1} - q_h^{n+1}\right\|_{L^2(0,T)} + \Delta t\|\partial_{tt}c\|_{L^2(t_n,t_{n+1};L^2(\Omega))}^2\\ &\quad + \Delta t\|\boldsymbol{u}_t\|_{L^2(t_n,t_{n+1};L^2(\Omega)^2)}^2 + \|\rho^{n+1}\|_{0,\Omega}^2 + (\Delta t)^{-1}\|\partial_t\rho\|_{L^2(t_n,t_{n+1};L^2(\Omega))}^2\\ &\quad + \left|\left|\left|\theta^{n+1}\right|\right|\right|_h^2 + \|\partial_t\theta^{n+1}\|_{0,\Omega}^2],\end{aligned} \tag{4.18}$$

and therefore it can be seen that

$$\tilde{A}_h(c_h^{n+1};\theta^{n+1},\partial_t\theta^{n+1}) \geq \frac{1}{2\Delta t}\left[\tilde{A}_h(c_h^{n+1};\theta^{n+1},\theta^{n+1}) - \tilde{A}_h(c_h^{n+1};\theta^n,\theta^n)\right]. \tag{4.19}$$

Summing over $n = 0,\dots,m-1$, using the equivalence between the norms $\|\cdot\|_{\eta_h}$ and $\|\cdot\|_{0,\Omega}$, the coercivity of the bilinear form $\tilde{A}_h(c_h^{n+1},\cdot,\cdot)$ and noting that $\theta^0 = 0$ in (4.18); we get that

$$\begin{aligned}\|\theta^m\|_h^2 \leq C\Delta t\sum_{n=0}^{m-1}[&\|c^{n+1}-c_h^{n+1}\|_{0,\Omega}^2 + \|\boldsymbol{u}^n - \boldsymbol{u}_h^n\|_{0,\Omega}^2 + \|q^{n+1}-q_h^{n+1}\|_{L^2(0,T)} \\ &+ \Delta t\|\partial_{tt}c\|^2_{L^2(t_n,t_{n+1};L^2(\Omega))} + \Delta t\|\boldsymbol{u}_t\|^2_{L^2(t_n,t_{n+1};L^2(\Omega)^2)} + \|\rho^{n+1}\|_{0,\Omega}^2 \\ &+ (\Delta t)^{-1}\|\partial_t\rho\|^2_{L^2(t_n,t_{n+1};L^2(\Omega))} + \|\theta^{n+1}\|_h^2],\end{aligned}$$

for an appropriate value of the constant C. Applying the discrete Gronwall's lemma and the estimates in Theorem 4.3, leads to the bound $\|\theta^m\|_h \leq C(h+\Delta t)$, which together with (4.12), implies that

$$\|c^m - c_h^m\|_h \leq C(h+\Delta t).$$

The bound for $\|c^{*m} - c_h^{*m}\|_h$ can be derived using the same approach. □

Appendix A. Proof of Theorem 4.2

Proof. At $t = t^m$ let the auxiliary functions $(\tilde{\boldsymbol{u}}_h^{*m},\tilde{p}_h^{*m})$ satisfy the following equations

$$\begin{aligned}(\alpha(c^m)\tilde{\boldsymbol{u}}_h^{*m},\boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h,\tilde{p}_h^{*m}) &= -(c^{*m}b(c^m)\nabla c^m,\boldsymbol{v}_h), \quad \forall\boldsymbol{v}_h\in U_h,\\ (\nabla\cdot\tilde{\boldsymbol{u}}_h^{*m},w_h) &= 0, \quad \forall w_h\in W_h.\end{aligned} \tag{A.1}$$

Then, using the Raviart–Thomas and L^2-projections (cf. [43,37]) we can assert that

$$\|\boldsymbol{u}^{*m} - \tilde{\boldsymbol{u}}_h^{*m}\|_{0,\Omega} + \|p^{*m}-\tilde{p}_h^{*m}\|_{0,\Omega} \leq Ch\left(\|\boldsymbol{u}^{*m}\|_{1,\Omega} + \|p^{*m}\|_{1,\Omega}\right). \tag{A.2}$$

Now, we split $\boldsymbol{u}^{*m} - \hat{\boldsymbol{u}}_h^{*m} = (\boldsymbol{u}^{*m} - \tilde{\boldsymbol{u}}_h^{*m}) + (\tilde{\boldsymbol{u}}_h^{*m} - \hat{\boldsymbol{u}}_h^{*m})$ and $p^{*m} - \hat{p}_h^{*m} = (p^{*m}-\tilde{p}_h^{*m}) + (\tilde{p}_h^{*m} - \hat{p}_h^{*m})$. Since the estimates of $\boldsymbol{u}^{*m} - \tilde{\boldsymbol{u}}_h^{*m}$ and $p^{*m}-\tilde{p}_h^{*m}$ are known from (A.2), it then suffices to estimate $\tilde{\boldsymbol{u}}_h^{*m} - \hat{\boldsymbol{u}}_h^{*m}$ and $\tilde{p}_h^{*m} - \hat{p}_h^{*m}$. Let $\tilde{\boldsymbol{e}}_{1h}^{*m} = \tilde{\boldsymbol{u}}_h^{*m} - \hat{\boldsymbol{u}}_h^{*m}$ and $\tilde{e}_{2h}^{*m} = \tilde{p}_h^{*m} - \hat{p}_h^{*m}$. Subtracting (4.3) from (A.1) we have

$$\begin{aligned}&(\alpha(\hat{c}_h^m)\tilde{\boldsymbol{e}}_{1h}^{*m},\gamma_h\boldsymbol{v}_h) - (\nabla\cdot\boldsymbol{v}_h,\tilde{e}_{2h}^{*m}) = [(\alpha(c^m)\tilde{\boldsymbol{u}}_h^{*m},\gamma_h\boldsymbol{v}_h - \boldsymbol{v}_h) + ((\alpha(\hat{c}_h^m)-\alpha(c^m))\tilde{\boldsymbol{u}}_h^{*m},\gamma_h\boldsymbol{v}_h)]\\ &\quad + [(c^{*m}b(c^m)\nabla c^m,\gamma_h\boldsymbol{v}_h - \boldsymbol{v}_h) + (\hat{c}_h^{*m}b(\hat{c}_h^m)\nabla\hat{c}_h^m - c^{*m}b(c^m)\nabla c^m,\gamma_h\boldsymbol{v}_h)], \ \forall\boldsymbol{v}_h\in U_h,\end{aligned} \tag{A.3}$$

$$\text{and} \quad (\nabla\cdot\tilde{\boldsymbol{e}}_{1h}^{*m},w_h) = 0, \quad \forall w_h\in W_h. \tag{A.4}$$

Since $\nabla\cdot U_h\subset W_h$, we take $w_h = \nabla\cdot\tilde{\boldsymbol{e}}_{1h}^{*m}$ in (A.4) to obtain $\|\nabla\cdot\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{0,\Omega} = 0$, which further implies (from the definition of $\|\cdot\|_{\mathrm{div},\Omega}$) that

$$\|\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{\mathrm{div},\Omega} = \|\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{0,\Omega}. \tag{A.5}$$

Choosing $\boldsymbol{v}_h = \tilde{\boldsymbol{e}}_{1h}^{*m}$ in (A.3) and $w_h = \tilde{e}_{2h}^{*m}$ in (A.4), we arrive at

$$\begin{aligned}C\|\tilde{\boldsymbol{e}}_{1h}^{*m}\|^2_{\mathrm{div},\Omega} \leq R_1 + R_2 &:= \left[(\alpha(c)\tilde{\boldsymbol{u}}_h^{*m},\gamma_h\tilde{\boldsymbol{e}}_{1h}^{*m} - \tilde{\boldsymbol{e}}_{1h}^{*m}) + ((\alpha(\hat{c}_h^m)-\alpha(c^m))\tilde{\boldsymbol{u}}_h^{*m},\gamma_h\tilde{\boldsymbol{e}}_{1h}^{*m})\right]\\ &+ \left[(c^{*m}b(c^m)\nabla c^m,\gamma_h\tilde{\boldsymbol{e}}_{1h}^{*m} - \tilde{\boldsymbol{e}}_{1h}^{*m}) + (\hat{c}_h^{*m}b(\hat{c}_h^m)\nabla\hat{c}_h^m - c^{*m}b(c^m)\nabla c^m,\gamma_h\tilde{\boldsymbol{e}}_{1h}^{*m})\right].\end{aligned} \tag{A.6}$$

Using then (3.3), the Lipschitz continuity of α, and (3.2), the first term in (A.6) can be bounded as

$$\begin{aligned}R_1 &\leq C\left(\|\tilde{\boldsymbol{u}}_h^{*m}\|_{0,\Omega}\|\tilde{\boldsymbol{e}}_{1h}^{*m} - \gamma_h\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{0,\Omega} + \|c^m-\hat{c}_h^m\|_{0,\Omega}\|\tilde{\boldsymbol{u}}_h^*\|_{L^\infty(\Omega)^2}\|\gamma_h\tilde{\boldsymbol{e}}_{1h}^*\|_{0,\Omega}\right)\\ &\leq C\left(h\|\tilde{\boldsymbol{u}}_h^*\|_{0,\Omega}\|\tilde{\boldsymbol{e}}_{1h}^*\|_{\mathrm{div},\Omega} + \|c-\hat{c}_h\|_{0,\Omega}\|\tilde{\boldsymbol{u}}_h^*\|_{L^\infty(\Omega)^2}\|\tilde{\boldsymbol{e}}_{1h}^*\|_{0,\Omega}\right).\end{aligned}$$

Regarding the second term in (A.6), we use (3.2) and (3.3) to obtain

$$\begin{aligned}R_2 \leq C(&h\|c^{*m}\|_{L^\infty(\Omega)}\|\nabla c^m\|_{L^\infty(\Omega)}\|\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{\mathrm{div},\Omega} + \|c^m - \hat{c}_h^m\|_{0,\Omega}\|\nabla\hat{c}_h^{*m}\|_{L^\infty(\Omega)}\|\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{0,\Omega}\\ &+ \|c^{*m}-\hat{c}_h^{*m}\|_{0,\Omega}\|\nabla c^m\|_{L^\infty(\Omega)}\|\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{0,\Omega}).\end{aligned}$$

Substituting these bounds back in (A.6), and using (A.5), we arrive at

$$\|\tilde{\boldsymbol{e}}_{1h}^{*m}\|_{0,\Omega} \leq C\left(\|c^m-\hat{c}_h^m\|_{0,\Omega} + \|c^{*m}-\hat{c}_h^{*m}\|_{0,\Omega}\right).$$

Next, to estimate $\left\|\tilde{e}_{2h}^{*m}\right\|$ we can choose $\boldsymbol{v}_h = \tilde{\boldsymbol{e}}_{1h}^{*m}$ in (A.3), leading to

$$(\nabla\cdot\tilde{\boldsymbol{e}}_{1h}^{*m},\tilde{e}_{2h}^{*m}) \le C\left[\left\|c^m-\hat{c}_h^m\right\|_{0,\Omega}+\left\|c^{*m}-\hat{c}_h^{*m}\right\|_{0,\Omega}+\left\|\tilde{\boldsymbol{e}}_{1h}^{*m}\right\|_{0,\Omega}\right]\left\|\tilde{\boldsymbol{e}}_{1h}^{*m}\right\|_{0,\Omega},$$

which, after applying the inf–sup condition, gives

$$\left\|\tilde{e}_{2h}^{*m}\right\|_{0,\Omega} \le C\left[\left\|c^m-\hat{c}_h^m\right\|_{0,\Omega}+\left\|c^{*m}-\hat{c}_h^{*m}\right\|_{0,\Omega}+\left\|\tilde{\boldsymbol{e}}_{1h}^{*m}\right\|_{0,\Omega}\right],$$

and so we have

$$\left\|\boldsymbol{u}^{*m}-\hat{\boldsymbol{u}}_h^{*m}\right\|_{L^2(\Omega)^2}+\left\|p^{*m}-\hat{p}_h^{*m}\right\|_{0,\Omega} \le C[\left\|c^m-\hat{c}_h^m\right\|_{0,\Omega}+\left\|c^{*m}-\hat{c}_h^{*m}\right\|_{0,\Omega}]. \tag{A.7}$$

Now, for a fixed $t = t^n$, let $\tilde{c}_h^{*n}$ denote the Riesz projection of c^{*n}. We then have that for any $z_h \in M_h$, the following condition holds

$$A_h(c^n;c^{*n}-\tilde{c}_h^{*n},z_h)-((b(c^n)\boldsymbol{u}^n-\mathcal{D}'(c^n)\nabla c^n)\cdot\nabla(c^{*n}-\tilde{c}_h^{*n}),z_h)+\lambda(c^{*n}-\tilde{c}_h^{*n},z_h)=0, \tag{A.8}$$

where $\lambda > 0$ is chosen such that, if fixing the first argument of the trilinear form in (A.8), the resulting bilinear form is coercive with respect to the norm $|||\cdot|||_h$. We then write $c^{*n}-\hat{c}_h^{*n}=(c^{*n}-\tilde{c}_h^{*n})+(\tilde{c}_h^{*n}-\hat{c}_h^{*n})=\rho^{*n}+\theta^{*n}$. Since the estimates for ρ^{*n} are known (see [13]), it only remains to derive bounds for θ^{*n}. We proceed to multiply (2.7) by $\eta_h z_h$, and integrating over Ω we have (at $t=t^{n+1}$)

$$\begin{aligned}&-(\phi\partial_t c^{*(n+1)},\eta_h z_h)-((b(c^{n+1})\boldsymbol{u}^{n+1}-\mathcal{D}'(c^{n+1})\nabla c^{n+1})\cdot\nabla c^{*(n+1)},\eta_h z_h)+A_h(c^{n+1};c^{*(n+1)},z_h)\\&\qquad+(\alpha'(c^{n+1})\boldsymbol{u}^{*(n+1)}\cdot\boldsymbol{u}^{n+1},\eta_h z_h)+(r_1q^{n+1}b(c^{n+1})c^{*(n+1)},\eta_h z_h)=(wc^{n+1},\eta_h z_h).\end{aligned} \tag{A.9}$$

Subtracting Eq. (4.4) from (A.9) yields

$$\begin{aligned}&-(\phi\frac{\theta^{*(n+1)}-\theta^{*n}}{\Delta t},\eta_h z_h)+A_h(c^{n+1};c^{*(n+1)},z_h)-A_h(\hat{c}_h^{n+1};\hat{c}_h^{*(n+1)},z_h)\\&-((b(c^{n+1})\boldsymbol{u}^{n+1}-\mathcal{D}'(c^{n+1})\nabla c^{n+1})\cdot\nabla c^{*(n+1)},\eta_h z_h)\\&+(r_1q^{n+1}\theta^{*(n+1)},\eta_h z_h)+((b(\hat{c}_h^{n+1})\hat{\boldsymbol{u}}_h^n-\mathcal{D}'(\hat{c}_h^{n+1})\nabla\hat{c}_h^{n+1})\cdot\nabla\hat{c}_h^{*(n+1)},\eta_h z_h)\\=&(\phi\frac{\rho^{*(n+1)}-\rho^{*n}}{\Delta t},\eta_h z_h)+\phi(\partial_t c^{*(n+1)}-\frac{c^{*(n+1)}-c^{*n}}{\Delta t},\eta_h z_h)\\&-(r_1q^{n+1}\rho^{*(n+1)},\eta_h z_h)-(r_1q^{n+1}c_h^{*(n+1)}(b(c^{n+1})-b(c_h^{n+1})),\eta_h z_h)\\&+(w(c^{n+1}-\hat{c}_h^{n+1}),\eta_h z_h)+(\alpha'(\hat{c}_h^{n+1})\hat{\boldsymbol{u}}_h^{*n}\cdot\hat{\boldsymbol{u}}_h^n-\alpha'(c^{n+1})\boldsymbol{u}^{*(n+1)}\cdot\boldsymbol{u}^{n+1},\eta_h z_h).\end{aligned}$$

Utilising relation (A.8) and choosing $z_h=\theta^{*(n+1)}$ in the previous equation, we can write

$$\begin{aligned}&-(\phi\frac{\theta^{*(n+1)}-\theta^{*n}}{\Delta t},\eta_h\theta^{*(n+1)})+A_h(\hat{c}_h^{n+1};\theta^{*(n+1)},\theta^{*(n+1)})-((b(c^{n+1})\boldsymbol{u}^{n+1}\\&-\mathcal{D}'(c^{n+1})\nabla c^{n+1})\cdot\nabla\theta^{*(n+1)},\eta_h\theta^{*(n+1)})+(r_1q^{n+1}\theta^{*(n+1)},\eta_h\theta^{*(n+1)})\\=&(\phi\frac{\rho^{*(n+1)}-\rho^{*n}}{\Delta t},\eta_h\theta^{*(n+1)})+\phi(\partial_t c^{*(n+1)}-\frac{c^{*(n+1)}-c^{*n}}{\Delta t},\eta_h\theta^{*(n+1)})\\&-(r_1q^{n+1}\rho^{*(n+1)},\eta_h\theta^{*(n+1)})-(\lambda\rho^{*(n+1)},\eta_h\theta^{*(n+1)})+(w(c^{n+1}-\hat{c}_h^{n+1}),\eta_h\theta^{*(n+1)})\\&-(r_1q^{n+1}c_h^{*(n+1)}(b(c^{n+1})-b(c_h^{n+1})),\eta_h\theta^{*(n+1)})+A_h(\hat{c}_h^{n+1};\tilde{c}_h^{*(n+1)},\theta^{*(n+1)})\\&+(\alpha'(\hat{c}_h^{n+1})\hat{\boldsymbol{u}}_h^{*n}\cdot\hat{\boldsymbol{u}}_h^n-\alpha'(c^{n+1})\boldsymbol{u}^{*(n+1)}\cdot\boldsymbol{u}^{n+1},\eta_h\theta^{*(n+1)})-A_h(c^{n+1};\tilde{c}_h^{*(n+1)},\theta^{*(n+1)})\\&+((b(\hat{c}_h^{n+1})\hat{\boldsymbol{u}}_h^n-\mathcal{D}'(\hat{c}_h^{n+1})\nabla\hat{c}_h^{n+1})\cdot\nabla\hat{c}_h^{*(n+1)},\theta^{*(n+1)}-\eta_h\theta^{*(n+1)})\\&-((b(c^{n+1})\boldsymbol{u}^{n+1}-\mathcal{D}'(c^{n+1})\nabla c^{n+1})\cdot\nabla c^{*(n+1)},\theta^{*(n+1)}-\eta_h\theta^{*(n+1)})\\&+((b(c^{n+1})\boldsymbol{u}^{n+1}-b(\hat{c}_h^{n+1})\hat{\boldsymbol{u}}_h^n+\mathcal{D}'(\hat{c}_h^{n+1})\nabla\hat{c}_h^{n+1}-\mathcal{D}'(c^{n+1})\nabla c^{n+1})\cdot\nabla\tilde{c}_h^{*(n+1)},\theta^{*(n+1)}).\end{aligned} \tag{A.10}$$

Then, thanks to Cauchy–Schwarz inequality and (3.7), we can deduce that

$$(\phi\frac{\rho^{*(n+1)}-\rho^{*n}}{\Delta t},\eta_h\theta^{*(n+1)}) \le C(\Delta t)^{-1/2}\left\|\partial_t\rho^*\right\|_{L^2(t_n,t_{n+1};L^2(\Omega))}\|\theta^{*(n+1)}\|_{0,\Omega},$$

and expanding in Taylor series it follows that

$$(\phi\partial_t c^{*(n+1)}-\phi\frac{c^{*(n+1)}-c^{*n}}{\Delta t},\eta_h\theta^{*(n+1)}) \le C\left(\Delta t\int_{t_n}^{t_{n+1}}\left\|\partial_{tt}c^*\right\|_{0,\Omega}^2 ds\right)^{1/2}\|\theta^{*(n+1)}\|_{0,\Omega}.$$

Next, exploiting similar arguments as in the proof of [28, Lemma 5.3], we can bound the terms in (A.10) and apply Young's inequality to obtain

$$\begin{aligned}
&-(\phi\frac{\theta^{*(n+1)}-\theta^{*n}}{\Delta t},\eta_h\theta^{*(n+1)})+A_h(\hat{c}_h^{n+1};\theta^{*(n+1)},\theta^{*(n+1)})\\
&\quad\leq C[\left\|c^{n+1}-\hat{c}_h^{n+1}\right\|_{0,\Omega}^2+\left\|\boldsymbol{u}^{*n}-\hat{\boldsymbol{u}}_h^{*n}\right\|_{0,\Omega}^2+\left\|\boldsymbol{u}^{n}-\hat{\boldsymbol{u}}_h^{n}\right\|_{0,\Omega}^2+\Delta t\left\|\partial_{tt}c^*\right\|_{L^2(t_n,t_{n+1};L^2(\Omega))}^2\\
&\qquad+\Delta t\|\boldsymbol{u}_t\|_{L^2(t_n,t_{n+1};L^2(\Omega)^2)}^2+\|\rho^{*(n+1)}\|_{0,\Omega}^2+(\Delta t)^{-1}\left\|\partial_t\rho^*\right\|_{L^2(t_n,t_{n+1};L^2(\Omega))}^2+\|\theta^{*(n+1)}\|_{0,\Omega}^2].
\end{aligned}\tag{A.11}$$

On the other hand, noting that $(\cdot,\eta_h\cdot)\geq 0$ allows us to write

$$-(\phi\frac{\theta^{*(n+1)}-\theta^{*n}}{\Delta t},\eta_h\theta^{*(n+1)})\geq\frac{\phi}{2\Delta t}\left[(\theta^{*n},\eta_h\theta^{*n})-(\theta^{*(n+1)},\eta_h\theta^{*(n+1)})\right].\tag{A.12}$$

Then, from (A.12) together with the coercivity of A_h and the definition of $|\!|\!|\cdot|\!|\!|_{\eta_h}$ in (A.11), we can sum over $n=m,\ldots,N-1$ to obtain

$$\begin{aligned}
|\!|\!|\theta^{*m}|\!|\!|_{\eta_h}^2\leq C\Delta t\sum_{n=m}^{N-1}&[\left\|c^{n+1}-\hat{c}_h^{n+1}\right\|_{0,\Omega}^2+\left\|\boldsymbol{u}^{*n}-\hat{\boldsymbol{u}}_h^{*n}\right\|_{0,\Omega}^2+\left\|\boldsymbol{u}^{n}-\hat{\boldsymbol{u}}_h^{n}\right\|_{0,\Omega}^2+\Delta t\left\|\partial_{tt}c^*\right\|_{L^2(0,T;L^2(\Omega))}^2\\
&+\Delta t\|\boldsymbol{u}_t\|_{L^2(0,T;L^2(\Omega)^2)}^2+\|\rho^{*(n+1)}\|_{0,\Omega}^2+(\Delta t)^{-1}\left\|\partial_t\rho^*\right\|_{L^2(0,T;L^2(\Omega))}^2+\|\theta^{*(n+1)}\|_{0,\Omega}^2].
\end{aligned}$$

Finally, we combine the discrete Gronwall's lemma, the equivalence of the norms $|\!|\!|\cdot|\!|\!|_{\eta_h}$ and $\|\cdot\|_{0,\Omega}$, Theorem 4.1, relation (A.7), and the available estimates for ρ^*, to obtain the bound $\|\theta^{*m}\|_{0,\Omega}\leq C(h+\Delta t)$, which in turn implies that

$$\left\|c^{*m}-\hat{c}_h^{*m}\right\|_{0,\Omega}\leq C(h+\Delta t).\tag{A.13}$$

Putting together (A.13) with the result from Theorem 4.1 in (A.7), we can also derive the estimate

$$\left\|\boldsymbol{u}^{*m}-\hat{\boldsymbol{u}}_h^{*m}\right\|_{0,\Omega}+\left\|p^{*m}-\hat{p}_h^{*m}\right\|_{0,\Omega}\leq C(h+\Delta t).\quad\square$$

Appendix B. Implementation of the optimal control solver

For sake of completeness of the presentation, we now proceed to describe the implementation of the numerical methods discussed in Section 3, and we stress that much of these steps can be found in [44–47].

Note that in the present applicative context, the profile evolution of the pressure field is expected to be much smoother than that of the saturation. We will therefore consider a first partition of J as $0=t_0<t_1<\cdots<t_M=T$ with step length $\Delta t_m=t_{m+1}-t_m$ dedicated for the Darcy equations, whereas for the saturation equation we take $0=t^0<t^1<\cdots<t_N=T$ with timestep $\Delta t^n=t^{n+1}-t^n$. We remark that such a splitting will still produce accurate approximations (see the discussion in e.g. [48]).

A splitting method for state and costate problems. To lighten the notation we will write

$$\begin{aligned}
&C^n=c_h(t^n),\quad C_m=c_h(t_m),\quad C^{*n}=c_h^*(t^n),\quad C_m^*=c_h^*(t_m),\\
&\mathbf{U}_m=\boldsymbol{u}_h(t_m),\quad P_m=p_h(t_m),\quad \mathbf{U}_m^*=\boldsymbol{u}_h^*(t_m),\quad P_m^*=p_h^*(t_m).
\end{aligned}$$

In addition, if $t_{m-1}<t^n\leq t_m$, then the velocity approximation at $t=t^n$ is defined by

$$\begin{aligned}
\mathbf{U}^n&=\left(1+\frac{t^n-t_{m-1}}{\Delta t_{m-2}}\right)\mathbf{U}_{m-1}-\frac{t^n-t_{m-1}}{\Delta t_{m-2}}\mathbf{U}_{m-2},\ \text{for } m=2,\ldots,M,\quad \mathbf{U}^n=\mathbf{U}_0,\quad\text{for } m=1,\\
\mathbf{U}^{*n}&=\left(1+\frac{t^n-t_{m-1}}{\Delta t_{m-2}}\right)\mathbf{U}_m^*-\frac{t^n-t_{m-1}}{\Delta t_{m-2}}\mathbf{U}_{m-1}^*,\ \text{for } m=M-1,\ldots,1,\quad \mathbf{U}^{n*}=\mathbf{U}_M,\ \text{for } m=M.
\end{aligned}$$

This allows us to recast (3.9)–(3.10) in the form: Find $(\mathbf{U},P):\{t_0,\ldots,t_M\}\to U_h\times W_h$ such that

$$\begin{aligned}
&(\alpha(C_m)\mathbf{U}_m,\gamma_h\boldsymbol{v}_h)-(\nabla\cdot\boldsymbol{v}_h,P_m)=0\quad\forall\boldsymbol{v}_h\in U_h,\\
&(\nabla\cdot\mathbf{U}_m,w_h)-((r_0-r_1)q_h^m,w_h)=0\quad\forall w_h\in W_h.
\end{aligned}\tag{B.1}$$

On the other hand, assuming a backward Euler approximation of the time derivative, the discrete state saturation equation (3.11) reduces to find $C:\{t^0,\ldots,t^N\}\to M_h$ such that

$$(\phi\frac{C^{n+1}-C^n}{\Delta t^n},\eta_hz_h)+A_h(C^{n+1};C^{n+1},z_h)+(b(C^{n+1})\mathbf{U}^{n+1}\cdot\nabla C^{n+1},\eta_hz_h)=(f(C^{n+1})r_0q_h^{i+1},\eta_hz_h).\tag{B.2}$$

For a given control q_h^0 we take $C^0 = C_0 = c_{0,h}$ and compute $(\mathbf{U}_0, P_0)$ from (B.1). Using $\mathbf{U}_0$ we can obtain C^1 from (B.2), and repeat the process throughout the time horizon. Then the discrete costate Darcy problem (3.12)–(3.13) consists in finding $(\mathbf{U}^*, P^*) : \{t_M, \ldots, t_0\} \to U_h \times W_h$ such that

$$(\alpha(C_m)\mathbf{U}_m^*, \gamma_h \boldsymbol{v}_h) - (\nabla \cdot \boldsymbol{v}_h, P_m^*) = -(C_m^* b(C_m)\nabla C_m, \gamma_h \boldsymbol{v}_h), \qquad (\nabla \cdot \mathbf{U}^{*m}, w_h) = 0. \tag{B.3}$$

The discrete costate saturation equation (3.14) reads: Find $C^* : \{t^N, \ldots, t^0\} \to M_h$ such that

$$\begin{aligned} -(\phi \frac{C^{*(n+1)} - C^{*n}}{\Delta t^n}, \eta_h z_h) + A_h(C^{n+1}; C^{*(n+1)}, z_h) - (b(C^{n+1})\mathbf{U}^{n+1} \cdot \nabla C^{*(n+1)}, \eta_h z_h) \\ + (\mathcal{D}'(C^{n+1})\nabla C^{n+1} \cdot \nabla C^{*(n+1)}, \eta_h z_h) + (\alpha'(C^{n+1})\mathbf{U}^{*(n+1)} \cdot \mathbf{U}^n, \eta_h z_h) \\ + (r_1 q_h^{n+1} b(C^{n+1})C^{*(n+1)}, \eta_h z_h) = (w C^{n+1}, \eta_h z_h). \end{aligned} \tag{B.4}$$

Using $C^{*N} = C_{*N} = 0$ we find $(\mathbf{U}_N^*, P_N^*)$ from (B.3) and using $\mathbf{U}_N^*$ we obtain C^{N-1} from (B.4). The process is then repeated down to $t = 0$.

Discrete problems in matrix form. Let $\{\boldsymbol{\Phi}_i\}_{j=1}^{N_m}$ be basis functions for the trial space U_h and $\{\chi_l^*\}_{l=1}^{N_e}$ denote characteristic functions for each element in $\mathcal{T}_h$, which form basis functions for W_h. We denote by N_m the number of midpoints of the edges in $\mathcal{T}_h$, and N_e stands for the total number of elements. The vectors containing the unknowns for each variable are then constructed as

$$\mathbf{U}_m = \sum_{j=1}^{N_m} \alpha_j^m \boldsymbol{\Phi}_j, \quad P_m = \sum_{l=1}^{N_e} \beta_l^m \chi_l^*, \quad \mathbf{U}_m^* = \sum_{j=1}^{N_m} \alpha_j^{*m} \boldsymbol{\Phi}_j, \quad P_m^* = \sum_{l=1}^{N_e} \beta_l^{*m} \chi_l^*,$$

where the coefficients are specified as

$$\alpha_j = (\boldsymbol{u}_h \cdot \boldsymbol{n}_j)(M_j), \quad \beta_l = p_h(b_{Kl}), \quad \alpha_j^* = (\boldsymbol{u}_h^* \cdot \boldsymbol{n}_j)(M_j), \quad \beta_l^* = p_h^*(b_{Kl}),$$

with b_{Kl} denoting the barycentre of the triangle K_l. After defining the following matrix and vector entries (with indexes $1 \le l \le N_e$, $1 \le i, j \le N_m$)

$$(A_m)_{ij} := \int_{T_{M_i}^*} \alpha(C_m)\boldsymbol{\Phi}_j \cdot \boldsymbol{\Phi}_i(M_i)\,\mathrm{d}\boldsymbol{x}, \quad (B_m)_{lj} := \int_{T_l} \nabla \cdot \boldsymbol{\Phi}_j\,\mathrm{d}\boldsymbol{x},$$

$$(F_m)_l := \int_{T_l} (r_0 - r_1)q_h^m\,\mathrm{d}\boldsymbol{x}, \quad (F_m^*)_i := -\int_{T_{M_i}^*} C_m^* b(C_m)\nabla C_m \cdot \boldsymbol{\Phi}_i(M_i)\,\mathrm{d}\boldsymbol{x},$$

we can write the matrix form of the discrete state Darcy equations (B.1) as

$$\begin{pmatrix} \mathbf{A}_m & \mathbf{B}_m \\ \mathbf{B}_m^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}^m \\ \boldsymbol{\beta}^m \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ \mathbf{F}_m \end{pmatrix}, \tag{B.5}$$

and the discrete costate Darcy problem (B.3) in matrix form as

$$\begin{pmatrix} \mathbf{A}_m & \mathbf{B}_m \\ \mathbf{B}_m^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \boldsymbol{\alpha}^{*m} \\ \boldsymbol{\beta}^{*m} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_m^* \\ \mathbf{0} \end{pmatrix}. \tag{B.6}$$

Regarding the transport equation, let $\{\Psi_i\}_{i=1}^{N_h}$ denote a basis for M_h, so that the vectors of state and costate saturations are $C^n = \sum_{i=1}^{N_h} \delta_i^n \Psi_i$ and $C^{*n} = \sum_{i=1}^{N_h} \delta_i^{*n} \Psi_i$. We denote $\boldsymbol{\delta}^n = (C^n(P_i))_{i=1}^{N_h}$ and $\boldsymbol{\delta}^{*n} = (C^{*n}(P_i))_{i=1}^{N_h}$, and define the following matrix and vector entries (with $1 \le i, j \le N_h$)

$$(D^n)_{ij} := \int_{K_i^*} \Psi_i \eta_h \Psi_j\,\mathrm{d}\boldsymbol{x}, \; (E_n)_{ij} := \int_{K_i^*} (b(C^n)\mathbf{U}^n \cdot \nabla \Psi_i)\eta_h \Psi_j\,\mathrm{d}\boldsymbol{x}, \; (G_n)_i := \int_{K_i^*} f(C^n) r_0 q_h^n \eta_h \Psi_i\,\mathrm{d}\boldsymbol{x},$$

$$(R_n)_{ij} := \int_{K_i^*} r_1 q_h^n b(C^n)\Psi_i \eta_h \Psi_j\,\mathrm{d}\boldsymbol{x}, \; (S^n)_{ij} := \int_{K_i^*} \mathcal{D}'(C^n)\nabla C^n \cdot \nabla \Psi_i \eta_h \Psi_j\,\mathrm{d}\boldsymbol{x},$$

$$(W_n)_i := \int_{K_i^*} w C^n \eta_h \Psi_i, \; (Z_n)_i := \int_{K_i^*} \alpha'(C^n)\mathbf{U}^n \cdot \mathbf{U}^{*n} \eta_h \Psi_i\,\mathrm{d}\boldsymbol{x}, \quad H_n := T_1^n + T_2^n + T_3^n + T_4^n,$$

$$(T_1^n)_{ij} = -\sum_{K \in \mathcal{T}_h} \sum_{k=1}^{3} \int_{v_{k+1} b_K v_k} \mathcal{D}(C^n)\nabla \Psi_i \cdot \boldsymbol{n} \eta_h \Psi_j\,\mathrm{d}s, \; (T_2^n)_{ij} = -\sum_{e \in \mathcal{E}_h} \int_e [\![\eta_h \Psi_i]\!] \cdot \langle \mathcal{D}(C^n)\nabla \Psi_j \rangle\,\mathrm{d}s,$$

$$(T_3^n)_{ij} = -\sum_{e \in \mathcal{E}_h} \int_e [\![\eta_h \Psi_j]\!] \cdot \langle \mathcal{D}(C^n)\nabla \Psi_i \rangle\,\mathrm{d}s, \quad (T_4^n)_{ij} = \sum_{e \in \mathcal{E}_h} \int_e \frac{\xi}{h_e} [\![\Psi_i]\!][\![\Psi_j]\!]\,\mathrm{d}s.$$

where v_k denotes a vertex of K.

Therefore the state saturation equation (B.2) adopts the following matrix form

$$\left[\phi \mathbf{D}^n + \Delta t_n(\mathbf{E}_n + \mathbf{H}_n)\right] \delta^{n+1} = \phi \mathbf{D}^n \delta^n + \Delta t_n \mathbf{G}^n, \tag{B.7}$$

and likewise, the matrix form of the costate saturation equation (B.4) reads

$$-\phi \mathbf{D}^n \delta^{*n} = \left[-\phi \mathbf{D}^n + \Delta t_n(-\mathbf{E}_n + \mathbf{H}_n + \mathbf{S}_n + \mathbf{R}_n)\right] \delta^{*(n+1)} - \Delta t_n(-\mathbf{Z}_n + \mathbf{W}_n). \tag{B.8}$$

Active set strategy. The control constraints can be implemented following the active set strategy adapted from [36,44], where the main steps of the method are be summarised in Algorithm 1,.

We first notice that a discrete variational inequality can be equivalently written as

$$q_h^n := \max\{0, \min\{\tilde{q}, -\alpha_0^{-1} \int_\Omega f(C^n) r_0 C^{*n} - (r_0 - r_1) P^{*n} \, \mathrm{d}\boldsymbol{x}\}\}, \;\; n = 0, \dots, N,$$

(see e.g. [28]), and we observe that the quantity $-\alpha_0^{-1} \int_\Omega f(C^n) r_0 C^{*n} - (r_0 - r_1) P^{*n} \, \mathrm{d}\boldsymbol{x}$ can be considered as a measure for the activity of control constraints. For each time horizon, we proceed to define the active sets $A_{k+1}^{-,n}$ and $A_{k+1}^{+,n}$ as well as inactive set I_{k+1}^n, at the current iteration, as follows

$$\begin{aligned}
A_{k+1}^{-,n} &:= \left\{x \in \Omega : -\alpha_0^{-1} \int_\Omega f(C_k^n) r_0 C_k^{*n} - (r_0 - r_1) P_k^{*n} \, \mathrm{d}\boldsymbol{x} < 0\right\}, \; n = 0, \dots, N, \\
A_{k+1}^{+,n} &:= \left\{x \in \Omega : -\alpha_0^{-1} \int_\Omega f(C_k^n) r_0 C_k^{*n} - (r_0 - r_1) P_k^{*n} \, \mathrm{d}\boldsymbol{x} > \tilde{q}\right\}, \; n = 0, \dots, N, \\
I_{k+1}^n &:= \Omega \setminus (A_{k+1}^{-,n} \cup A_{k+1}^{+,n}),
\end{aligned}$$

then we have

$$q_{h,k+1}^n = \tilde{q} \chi_{A_{k+1}^{+,n}} - \alpha_0^{-1} \int_\Omega f(C_k^n) r_0 C_k^{*n} - (r_0 - r_1) P_k^{*n} (1 - \chi_{A_{k+1}^{-,n}} - \chi_{A_{k+1}^{+,n}}), \tag{B.9}$$

where $\chi_{A_{k+1}^{-,n}}$ and $\chi_{A_{k+1}^{+,n}}$ are the characteristic functions corresponding to the active sets $A_{k+1}^{-,n}$ and $A_{k+1}^{+,n}$, respectively. Using the value of C, C^* and P^*, we can compute the discrete control q_h for each time horizon and the process is repeated until reaching the termination criteria.

Algorithm 1 Method of active sets

1: Choose **and** store arbitrary initial guess $q_{h,0}$ **and** set $k = 0$
2: **for** $k = 0, 1, \dots,$ **do**
3: Given the control $q_{h,k}$, **compute** $(\mathbf{U}_k, P_k) : \{t_0, t_1, \dots, t_M\} \to U_h \times W_h$ from (B.5)
4: **compute** $C_k : \{t^0, t^1, \dots, t^N\} \to M_h$ from (B.7)
5: **compute** $(\mathbf{U}_k^*, P_k^*) : \{t_M, t_{M-1}, \dots, t_0\} \to U_h \times W_h$ from (B.6)
6: **compute** $C_k^* : \{t^N, t^{N-1}, \dots, t^0\} \to M_h$ from (B.8)
7: Update $q_{h,k} \leftarrow q_{h,k+1}$ from relation (B.9)
8: **if** $A_{k+1}^- = A_k^-$ **and** $A_{k+1}^+ = A_k^+$ **then**
9: **stop**
10: **else**
11: **go to** step 3
12: **end if**
13: **end for**

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