Formulation and analysis of fully-mixed methods for stress-assisted diffusion problems

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ABSTRACT

This paper is devoted to the mathematical and numerical analysis of a mixed-mixed PDE system describing the stress-assisted diffusion of a solute into an elastic material. The equations of elastostatics are written in mixed form using stress, rotation and displacements, whereas the diffusion equation is also set in a mixed three-field form, solving for the solute concentration, its gradient, and the diffusive flux. This setting simplifies the treatment of the nonlinearity in the stress-assisted diffusion term. The analysis of existence and uniqueness of weak solutions to the coupled problem follows as a combination of Schauder and Banach fixed-point theorems together with the Babuška–Brezzi and Lax–Milgram theories. Concerning numerical discretization, we propose two families of finite element methods, based on either PEERS or Arnold–Falk–Winther elements for elasticity, and a Raviart–Thomas and piecewise polynomial triplet approximating the mixed diffusion equation. We prove the well-posedness of the discrete problems, and derive optimal error bounds using a Strang inequality. We further confirm the accuracy and performance of our methods through computational tests.

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1. Introduction

We are interested in the mathematical and numerical study of a stationary problem representing diffusion–deformation processes where the stress acts as a coupling variable. So-called stress-assisted diffusion models (derived from thermodynamic principles and phenomenological arguments in e.g. [1,2]) are relevant to numerous applications including diffusion of boron and arsenic in silicon [3], hydrogen diffusion in metals [4], voiding of aluminium conductor lines in integrated circuits [5], strain-aging measurements in iron [6], sorption in polymers [7], to name a few. Of special appeal to us is the study of microscopic electrode damage in lithium ion batteries [8–12]. When lithium diffuses into a secondary particle (an anode made of e.g. silicon), its core expands and its elastic response, also with that of neighbouring particles and the surrounding electrolyte, modify the diffusive properties inside the medium. If the process is confined inside the anode, then the electric field is practically constant and the system may be described solely in terms of diffusion and stress.

Regarding the mathematical and numerical analysis of related models, the literature is rather scarce. Some recent references include homogenization of concentration–electric potential systems [13], multiscale analysis of the deterioration

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of binder in electrodes [14], and a general local–global well-posedness theory [15]. Differently from these approaches, in [16] we have recently proposed a mixed-primal formulation for stress-assisted diffusion. The model covers the linear elastic regime, it incorporates the rotation tensor as supplementary variable serving to impose stress symmetry in a weak manner; and this mixed problem is coupled with a primal formulation for diffusion. Here, in contrast, we consider an augmented mixed formulation for the diffusion equation. Similarly to [17], the concentration gradient and the diffusive flux are incorporated as auxiliary unknowns, which allows us to treat the stress-dependent diffusivity using a dual-mixed setting. In order to apply the regularity estimates from [16], we augment the formulation with redundant terms arising from a constitutive equation. Next, following the approach introduced in [18], we combine fixed-point arguments, regularity estimates, the Babuška–Brezzi theory, the Lax–Milgram lemma, the Sobolev embedding and Rellich–Kondrachov theorems, and small data assumptions to establish existence and uniqueness of solution of the continuous problem. The solvability of the Galerkin scheme follows from the Brouwer fixed-point theorem and properties of the finite element subspaces. Finally, the convergence analysis is conducted adapting Strang inequalities, Céa estimates, and using approximation properties of the finite element spaces.

The rest of the paper is organized as follows. In Section 2 we describe required notation and functional spaces to be employed along the paper. Then, we introduce the model problem and requirements on the specific constitutive functions. Next, in Section 3 we derive the augmented fully-mixed formulation and establish its well-posedness. The Galerkin scheme and the existence of discrete solution are then studied in Section 4. In addition, under similar assumptions we deduce error bounds in Section 5; and we close in Section 6 with a numerical example that confirms the theoretical rates of convergence, and a second test studying the applicability of the discrete formulation in the simulation of 3D microscopic lithiation processes.

2. The model problem

Let \( \Omega \subseteq \mathbb{R}^n, n \in \{2, 3\} \), be a given bounded domain with polyhedral boundary \( \Gamma = \partial \Omega \) and denote by \( r \) the outward unit normal vector on the whole boundary \( \partial \Omega \). Standard notation will be adopted for Lebesgue spaces \( L^p(\Omega) \) and Sobolev spaces \( H^1(\Omega) \) with norms \( \| \cdot \|_{L^p(\Omega)} \) and seminorms \( | \cdot |_{L^p(\Omega)} \). In particular, \( H^{1/2}(\Gamma) \) is the space of traces of functions of \( H^1(\Omega) \), while \( H^{-1/2}(\Gamma) \) denotes its dual. By \( | \cdot | \) we will denote both the Euclidean norm in \( \mathbb{R}^n \) and the Frobenius norm in \( \mathbb{R}^{n \times n} \). Let \( \mathbf{div} \) be the divergence operator acting along the rows of the tensor \( \tau \). We recall that the tensorial \( H(\mathbf{div}) \) space

\[
H(\mathbf{div}; \Omega) := \{ \tau \in L^2(\Omega) : \mathbf{div} \tau \in L^2(\Omega) \} ,
\]
equipped with the norm \( \| \tau \|_{H(\mathbf{div}; \Omega)} := \| \tau \|_{L^2(\Omega)}^2 + \| \mathbf{div} \tau \|_{L^2(\Omega)}^2 \). For any tensors \( \tau = (\tau_{ij})_{i,j=1,n} \), and \( l : (\tau_{ij})_{i,j=1,n} \), we denote the transpose, trace, tensor product, and deviatoric tensor, respectively, as

\[
\tau^\top := (\tau_{ij})_{j=1,n}, \quad \mathbf{tr}(\tau) := \sum_{i=1}^n \tau_{ii} \quad \tau : \xi := \sum_{i,j=1}^n \tau_{ij} \xi_{ij}, \quad \text{and} \quad \tau^d := \tau - \frac{1}{n} \mathbf{tr}(\tau) I.
\]

Finally, we will denote by \( \| \cdot \|_{L^\infty(\Omega)} \) the norm of the Banach space \( L^\infty(\Omega) \) as well as of its vectorial version \( L^\infty(\Omega) \).

Let us consider the following system of PDEs, governing the diffusion of a solute interacting with the motion of an elastic solid occupying the domain \( \Omega \):

\[
\begin{align*}
\sigma &= \lambda \mathbf{tr}(\mathbf{u}) I + 2 \mu \mathbf{e}(\mathbf{u}) \quad \text{in} \ \Omega, & -\mathbf{div} \sigma &= \mathbf{f}(\phi) \quad \text{in} \ \Omega, \\
\tilde{\sigma} &= \partial(\sigma) \nabla \phi \quad \text{in} \ \Omega, & -\mathbf{div} \tilde{\sigma} &= \mathbf{g}(\mathbf{u}) \quad \text{in} \ \Omega, \\
\mathbf{u} &= \mathbf{u}_0 \quad \text{on} \ \Gamma, & \phi &= \phi_0 \quad \text{on} \ \Gamma.
\end{align*}
\]

Eq. (2.1) states the constitutive relation and momentum balance for the elasticity equations, problem (2.2) defines the diffusion equation and diffusive flux, and (2.3) specifies the Dirichlet boundary conditions \( \mathbf{u}_0 \in H^{1/2}(\Gamma) \) and \( \phi_0 \in H^{1/2}(\Gamma) \). The involved quantities and model parameters are the Cauchy solid stress \( \sigma \), the displacement field \( \mathbf{u} \), the infinitesimal strain tensor \( \mathbf{e}(\mathbf{u}) := \frac{1}{2} (\nabla \mathbf{u} + \nabla \mathbf{u}^\top) \), the Lamé constants \( \lambda, \mu > 0 \) characterizing the material, the diffusive flux \( \tilde{\sigma} \), the solute concentration \( \phi \), the tensorial diffusivity \( \partial : \mathbb{R}^{n \times n} \to \mathbb{R}^{n \times n} \), the vector of body loads \( \mathbf{f} : \mathbb{R} \to \mathbb{R}^n \), and a displacement-dependent source term \( \mathbf{g} : \mathbb{R}^n \to \mathbb{R} \). For the load, source, and diffusivity functions we will require uniform boundedness and Lipschitz continuity, that is there exist positive constants \( f_1, f_2, f_3, g_1, g_2, L_\phi, \) and \( \partial_1, \partial_2, L_\partial \), such that

\[
\begin{align*}
f_1 \leq \| f(s) \| & \leq f_2, \quad \| f(s) - f(t) \| \leq L_f | s - t | \quad \forall s, t \in \mathbb{R}, \\
g_1 \leq \| \mathbf{g}(\mathbf{w}) \| & \leq g_2, \quad \| \mathbf{g}(\mathbf{v}) - \mathbf{g}(\mathbf{w}) \| \leq L_g | \mathbf{v} - \mathbf{w} | \quad \forall \mathbf{v}, \mathbf{w} \in \mathbb{R}^n, \\
\partial_1 \leq | \partial(\tau) | & \leq \partial_2, \quad | \partial(\tau - \partial(\xi)) | \leq L_\partial | \tau - \xi | \quad \forall \tau, \xi \in \mathbb{R}^{n \times n}.
\end{align*}
\]

Additionally, \( \partial \) is of class \( C^1 \) and uniformly positive definite, the latter meaning that there exists \( \partial_0 > 0 \) such that

\[
\partial(\tau) \mathbf{w} \cdot \mathbf{w} \geq \partial_0 | \mathbf{w} |^2 \quad \forall \mathbf{w} \in \mathbb{R}^n, \quad \forall \tau \in \mathbb{R}^{n \times n}.
\]
Finally, we assume that $f(\phi) \in H^1(\Omega)$ for each $\phi \in H^1(\Omega)$, and that for each $\gamma \in (0, 1)$ there exists a constant $C_\gamma > 0$ such that $g(w) \in H^\gamma(\Omega)$ for each $w \in H^\gamma(\Omega)$ and

$$
\|g(w)\|_{\gamma, \Omega} \leq C_\gamma \|w\|_{\gamma, \Omega}.
$$

(2.8)

Examples of stress-dependent diffusivity functions and concentration-dependent body loads may include exponential functions of the volumetric stress for lithiation of batteries [10], simple polynomial relationships for biological materials [19], or Carreau-type laws for $\vartheta$, that is

$$
\vartheta(\sigma) = C_0 \exp(-\text{tr} \sigma) I, \quad \vartheta(\sigma) = C_0 I + C_1 \sigma + C_2 \sigma^2, \quad \vartheta(\sigma) = (C_0 + C_1(1 - |\sigma|^2)^{-1/2}) I,
$$

respectively, where $C_0, C_1, C_2$ are constants, whereas for $f$ linear dependences modelling isotropic swelling in composite materials [20], saturation-based descriptions for viscous layers [21], or concentration gradient modulations for single-cell mechanics [22] are considered, that is

$$
f(\phi) = C \phi, \quad f(\phi) = C(1 - \phi)^{m-1}, \quad f(\phi) = C_0 \nabla \phi,
$$

respectively, where $C \in \mathbb{R}^n$ and $m > 1$. Nevertheless, not all of these fulfil each one of the above described hypotheses. For instance, the constitutive equation for diffusivity $\vartheta(\sigma) = C_0 I + C_1 \sigma + C_2 \sigma^2$ violates (2.6) and it is not necessarily satisfying (2.7) for certain stress configurations. Illustrations of the latter issue are discussed in [19].

3. Weak formulation and solvability analysis

In this section we derive an augmented fully-mixed variational formulation for (2.1)–(2.3) and propose a fixed-point strategy for its analysis. We show that the fixed-point operator is well-defined and apply the Schauder’s theorem to prove existence of solution, whereas Banach fixed-point theorem will lead to uniqueness of solution under small data assumptions.

3.1. The mixed-mixed formulation

We begin by recalling from [23] that $H^1(\Omega; \Omega) = H^1(div; \Omega) \oplus \mathbb{R}I$, with

$$
H^1(div; \Omega) := \left\{ \tau \in H(div; \Omega) : \int_\Omega \text{tr}(\tau) = 0 \right\},
$$

which means that for each $\tau \in H(div; \Omega)$ there exist unique

$$
\tau_0 := \tau - \left\{ \frac{1}{|\Omega|} \int_\Omega \text{tr}(\tau) \right\} I \in H^1(div; \Omega)
$$

and $d := \frac{1}{|\Omega|} \int_\Omega \text{tr}(\tau) \in \mathbb{R},$

such that $\tau = \tau_0 + d I$. Also, we define the space of skew-symmetric tensors as

$$
L^2_{\text{skew}}(\Omega) := \{ \eta \in L^2(\Omega) : \eta + \eta^T = 0 \}.
$$

Then, proceeding as in [16, Section 2.1], we apply the Dirichlet boundary condition for displacements (first relation of (2.3)) and the aforementioned orthogonal decomposition to write the elasticity problem in weak form: find $(\sigma, (u, \rho)) \in H_1 := H^1(div; \Omega) \times (L^2(\Omega) \times L^2_{\text{skew}}(\Omega))$ such that

$$
a(\sigma, \tau) + b(\tau, (u, \rho)) = G(\tau) \quad \forall \tau \in H^1(div; \Omega),
$$

$$
b(\sigma, (v, \eta)) = F_\sigma(v, \eta) \quad \forall (v, \eta) \in L^2(\Omega) \times L^2_{\text{skew}}(\Omega),
$$

(3.1)

where $a : H^1(div; \Omega) \times H^1(div; \Omega) \to \mathbb{R}$ and $b : H^1(div; \Omega) \times (L^2(\Omega) \times L^2_{\text{skew}}(\Omega)) \to \mathbb{R}$ are bilinear forms defined as

$$
a(\xi, \tau) = \frac{1}{2\mu} \int_\Omega \tau^T : \xi d\Omega + \frac{1}{n(n+2\mu)} \int_\Omega \text{tr}(\xi) \text{tr}(\tau), \quad b(\tau, (v, \eta)) := \int_\Omega v \cdot \nabla \tau + \int_\Omega \eta : \tau,
$$

for $\xi, \tau \in H^1(div; \Omega)$ and $(v, \eta) \in L^2(\Omega) \times L^2_{\text{skew}}(\Omega)$. In turn, the functionals $F_\phi \in (L^2(\Omega) \times L^2_{\text{skew}}(\Omega))^\prime$ and $G \in H^1(div; \Omega)^\prime$ are given by

$$
G(\tau) := \langle \tau v, u_0 \rangle \Gamma \quad \text{and} \quad F_\phi(v, \eta) := -\int_\Omega f(\phi) \cdot v,
$$

(3.2)

for $(\tau, (v, \eta)) \in H_1$, where $\langle \cdot, \cdot \rangle_\Gamma$ stands for the duality pairing of $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$. Details on the derivation of the weak formulation (3.1) can be found in [24] as well as in [25].

In turn, defining the concentration gradient $\mathbf{t} := \nabla \phi$, we can recast the diffusion equation as

$$
\tilde{\sigma} = \vartheta(\sigma) \mathbf{t} \quad \text{in} \quad \Omega, \quad \mathbf{t} = \nabla \phi \quad \text{in} \quad \Omega, \quad -\text{div} \tilde{\sigma} = g(u) \quad \text{in} \quad \Omega,
$$

$$
\phi = \phi_0 \quad \text{on} \quad \Gamma.
$$

(3.3)
We then test the three-field problem (3.3) against \( s \in L^2(\Omega) \), \( \tilde{\tau} \in H(\text{div}; \Omega) \) and \( \psi \in L^2(\Omega) \). Integrating by parts the expression \( \int_{\Omega} \nabla \phi \cdot \tilde{\tau} \) and using the Dirichlet boundary condition for \( \phi \) (second equation in (2.3)), we arrive at the weak formulation: find \((t, \tilde{\sigma}, \phi) \in L^2(\Omega) \times H(\text{div}; \Omega) \times L^2(\Omega)\) such that
\[
\int_{\Omega} \tilde{\tau} \cdot t - \int_{\Omega} \tilde{\sigma} \cdot s = 0 \quad \forall s \in L^2(\Omega),
\]
\[
\int_{\Omega} \phi \text{div} \tilde{\tau} = (\tilde{\tau} \cdot v, \phi_D) \quad \forall \tilde{\tau} \in H(\text{div}; \Omega),
\]
\[
- \int_{\Omega} \psi \text{div} \tilde{\sigma} = \int_{\Omega} g(u) \quad \forall \psi \in L^2(\Omega).
\]
In view of modifying the regularity properties of the coupled problem, we proceed to enrich the foregoing equations with the following residual terms:
\[
\kappa_1 \int_{\Omega} \{ \tilde{\sigma} - \theta(\sigma) t \} \cdot \tilde{\tau} = 0 \quad \forall \tilde{\tau} \in H(\text{div}; \Omega),
\]
\[
\kappa_2 \int_{\Omega} \text{div} \tilde{\sigma} \text{div} \tilde{\tau} = - \kappa_2 \int_{\Omega} g(u) \text{div} \tilde{\tau} \quad \forall \tilde{\tau} \in H(\text{div}; \Omega),
\]
\[
\kappa_3 \int_{\Omega} \{ \nabla \phi - t \} \cdot \nabla \psi = 0 \quad \forall \psi \in H^1(\Omega),
\]
\[
\kappa_4 \int_{\Gamma} \phi \psi = \kappa_4 \int_{\Gamma} \phi_D \psi \quad \forall \psi \in H^1(\Omega),
\]
where \( \kappa_1, \kappa_2, \kappa_3 \) and \( \kappa_4 \) are positive parameters to be specified later on. We remark that the identities required in (3.5) are nothing but the constitutive and the equilibrium equations concerning \( \tilde{\sigma} \), along with the relation defining \( t \), and the Dirichlet boundary condition for \( \phi \); all of them tested differently from (3.4). Instead of (3.4), we will now focus on the following augmented formulation for the diffusion problem: find \((t, \tilde{\sigma}, \phi) \in H_2 := L^2(\Omega) \times H(\text{div}; \Omega) \times H^1(\Omega)\) such that
\[
A_u((t, \tilde{\sigma}, \phi), (s, \tilde{\tau}, \psi)) = G_u(s, \tilde{\tau}, \psi) \quad \forall (s, \tilde{\tau}, \psi) \in H_2,
\]
where
\[
A_u((t, \tilde{\sigma}, \phi), (s, \tilde{\tau}, \psi)) := \int_{\Omega} \theta(\sigma) t \cdot s - \int_{\Omega} \tilde{\sigma} \cdot s + \int_{\Omega} \tilde{\tau} \cdot t + \int_{\Omega} \phi \text{div} \tilde{\tau} - \int_{\Omega} \psi \text{div} \tilde{\sigma}
\]
\[
+ \kappa_1 \int_{\Omega} \{ \tilde{\sigma} - \theta(\sigma) t \} \cdot \tilde{\tau} + \kappa_2 \int_{\Omega} \text{div} \tilde{\sigma} \text{div} \tilde{\tau} + \kappa_3 \int_{\Omega} \{ \nabla \phi - t \} \cdot \nabla \psi + \kappa_4 \int_{\Gamma} \phi \psi,
\]
and
\[
G_u(s, \tilde{\tau}, \psi) := (\tilde{\tau} \cdot v, \phi_D) + \int_{\Omega} \psi g(u) - \kappa_2 \int_{\Omega} g(u) \text{div} \tilde{\tau} + \kappa_4 \int_{\Gamma} \phi_D \psi.
\]
Consequently, we arrive at the following augmented fully-mixed formulation for (2.1)--(2.3): find \((\sigma, (u, \rho)), (t, \tilde{\sigma}, \phi) \in H_1 \times H_2\) such that
\[
a(\sigma, \tau) + b(\tau, (u, \rho)) = G(\tau) \quad \forall \tau \in H_0(\text{div}; \Omega),
\]
\[
b(\sigma, (v, \eta)) = F_\rho(v, \eta) \quad \forall (v, \eta) \in L^2(\Omega) \times L^2(\Omega),
\]
\[
A_u((t, \tilde{\sigma}, \phi), (s, \tilde{\tau}, \psi)) = G_u(s, \tilde{\tau}, \psi) \quad \forall (s, \tilde{\tau}, \psi) \in H_2.
\]

### 3.2. A fixed-point approach

Here we utilize a fixed-point strategy to prove that problem (3.9) is well-posed. Let us first define the operator \( S : H^1(\Omega) \to H_1 \) as
\[
S(\phi) := (S_1(\phi), (S_2(\phi), S_3(\phi))) := (\sigma, (u, \rho)) \quad \forall \phi \in H^1(\Omega),
\]
where \((\sigma, (u, \rho))\) is the unique solution of (3.1) with the given \( \phi \). In turn, we define the operator \( \tilde{S} : H_0(\text{div}; \Omega) \times L^2(\Omega) \to H_2 \) as
\[
\tilde{S}(\sigma, u) := (\tilde{S}_1(\sigma, u), \tilde{S}_2(\sigma, u), \tilde{S}_3(\sigma, u)) := (t, \tilde{\sigma}, \phi) \quad \forall (\sigma, u) \in H_0(\text{div}; \Omega) \times L^2(\Omega),
\]
where \((t, \tilde{\sigma}, \phi)\) is the unique solution of (3.6) with the given \((\sigma, u)\). In this way, by introducing the operator \( T : H^1(\Omega) \to H^1(\Omega) \) as
\[
T(\phi) := \tilde{S}_3(S_1(\phi), S_2(\phi)) \quad \forall \phi \in H^1(\Omega),
\]
we realize that (3.9) can be rewritten as the fixed-point problem: find $\phi \in H^1(\Omega)$ such that

$$T(\phi) = \phi.$$  \hfill (3.10)

However, we remark in advance that the definition of $T$ will be only in a closed ball of $H^1(\Omega)$.

We also collect the following two technical lemmas, whose proofs can be found in [24, Lemma 2.3], and [26, Lemma 3.3], respectively.

**Lemma 3.1.** There exists $c_1 > 0$ such that

$$c_1 \|\tau\|_{0, \Omega}^2 \leq \|\div \tau\|_{0, \Omega}^2 + \|\nabla \tau\|_{0, \Omega}^2 \quad \forall \tau \in H^1_0(\div; \Omega).$$

**Lemma 3.2.** There exists $c_2 > 0$ such that

$$|\nabla (\tau) + \psi \nabla \tau| \leq c_2 \|\psi\|_{1, \Omega} \quad \forall \psi \in H^1(\Omega).$$

In what follows we show that $T$ has at least one fixed point. Firstly we will prove that the uncoupled problems defined by $S$ and $\tilde{S}$ are well-posed, where we emphasize that $\tilde{S}$ is defined similarly as in [16], and therefore we omit parts of the proofs whenever necessary. Our analysis will focus on the uncoupled problem (3.6) and its repercussion on $T$. Let us start by recalling the continuity of $a$ and $b$. For a proof we refer to e.g. [24].

$$|a(\eta, \tau)| \leq \frac{1}{\mu} \|\eta\|_{\div, \Omega} \|\tau\|_{\div, \Omega} \quad \forall \eta, \tau \in H^1_0(\div; \Omega),$$

$$|b(\eta, (\tau, \psi))| \leq \|\eta\|_{\div, \Omega} \|\tau, \psi\| \quad \forall \tau, \psi \in H^1_0(\div; \Omega), \quad \forall (\tau, \psi) \in L^2(\Omega) \times L^2_{\text{skew}}(\Omega).$$

Furthermore, it is not difficult to see that $a$ is strongly elliptic in the kernel of $b$. In fact, we denote the operator induced by the bilinear form $b$ as $B$, and note that

$$V := \text{Ker}(B) = \{ \tau \in H^1_0(\div; \Omega) : \div \tau = 0 \text{ in } \Omega, \quad \tau = \tau^1 \text{ in } \Omega \},$$

from which, we deduce that

$$a(\eta, \tau) \geq \frac{1}{2\mu} \|\eta\|_{0, \Omega}^2 \geq \frac{c_1}{2\mu} \|\eta\|_{0, \Omega}^2 = \alpha \|\eta\|_{\div, \Omega}^2 \quad \forall \eta \in V,$$

where $c_1$ is the constant provided by Lemma 3.1. Additionally, as a slight modification of the proof of [24, Section 2.4.3], we find that $B$ is surjective. Finally, we observe that $G$ and $F_\phi$ are bounded with

$$\|G\| \leq \|u_0\|_{1/2, R} \quad \text{and} \quad \|F_\phi\| \leq f_2|\Omega|^{1/2}.$$  \hfill (3.13)

This analysis confirms the well-posedness of (3.1), which is abridged in the following lemma.

**Lemma 3.3.** For each $\phi \in H^1(\Omega)$ the problem (3.1) has a unique solution $S(\phi) := (\sigma, (u, \rho)) \in H_1$. Moreover, there exists $c_5 > 0$, independent of $\phi$, such that

$$\|S(\phi)\|_{H_1} = \|\sigma, (u, \rho)\|_{H_1} \leq c_5 \left\{ \|u_0\|_{1/2, R} + f_2|\Omega|^{1/2} \right\}.$$  \hfill (3.14)

**Proof.** It follows from estimates (3.11)–(3.13) and a direct application of the Babuška–Brezzi theory (see, e.g. [23] and [24, Thm. 2.3]). We refer to [16, Lemma 2.2] for further details.

In turn, we prove the well-posedness of problem (3.6) with the next result.

**Lemma 3.4.** Assume that $\kappa_1 \in \left(0, \frac{2\alpha_0}{\beta_0^2}\right)$ and $\kappa_2, \kappa_3 \in \left(0, \frac{2\delta}{\beta_0^2}\right)$ with $\delta \in \left(0, \frac{1}{2}\right) \supset \delta \in (0, 2)$, and $\kappa_2, \kappa_4 > 0$. Then, for each $(\sigma, u) \in H^1_0(\div; \Omega) \times L^2(\Omega)$, problem (3.6) has a unique solution $\tilde{S}(\sigma, u) = (\tilde{\sigma}, \tilde{\phi}) \in H_2$. Moreover, there exists $c_5 > 0$, independent of $(\sigma, u)$, such that

$$\|\tilde{S}(\sigma, u)\|_{H_2} = \|(\tilde{\sigma}, \tilde{\phi})\|_{H_2} \leq c_5 \left\{ \|\phi_0\|_{1/2, R} + g_2|\Omega|^{1/2} \right\}.$$  \hfill (3.15)

**Proof.** Firstly, we note from (3.7) that $A_\phi$ is a bilinear form. Next, applying Cauchy–Schwarz’s inequality, the upper bound for $\partial$ (cf. (2.6)), and the trace theorem (with constant $c_0$), we find that

$$|A_\phi((\tilde{\sigma}, \tilde{\phi}, (s, \tilde{\tau}, \psi))| \leq \delta_2 |\tilde{\sigma}|_{0, \Omega} |s|_{0, \Omega} + \tilde{\sigma} |\tilde{\tau}|_{0, \Omega} + |\nabla \tilde{\tau}|_{0, \Omega} + \kappa_1 |\tilde{\tau}|_{0, \Omega} + k_1 |\tilde{\tau}|_{0, \Omega} + k_2 |\tilde{\tau}|_{0, \Omega} + |\nabla \tilde{\tau}|_{0, \Omega} + k_3 |\tilde{\tau}|_{0, \Omega} + k_3 |\tilde{\tau}|_{0, \Omega} + k_3 |\tilde{\tau}|_{0, \Omega} + |\nabla \tilde{\tau}|_{0, \Omega} + k_3 |\tilde{\tau}|_{0, \Omega} + k_3 |\tilde{\tau}|_{0, \Omega} + k_3 |\tilde{\tau}|_{0, \Omega} + k_3 |\tilde{\tau}|_{0, \Omega}.$$

It follows that there exists a positive constant $\|A\|$, depending on $\delta_2, c_0, \kappa_1, k_2, k_3$ and $k_4$, such that

$$|A_\phi((\tilde{\sigma}, \tilde{\phi}, (s, \tilde{\tau}, \psi))| \leq \|A\| \|(|\tilde{\sigma}, \tilde{\phi}, (s, \tilde{\tau}, \psi))\|_{H_2} \quad \forall (\tilde{\sigma}, \tilde{\phi}, (s, \tilde{\tau}, \psi) \in H_2,$$  \hfill (3.16)
and hence $A_\sigma$ is bounded independently of $(\sigma, u) \in H_0(\text{div}; \Omega) \times L^2(\Omega)$. In turn, we now aim to show that $A_\sigma$ is $H_2$-elliptic. To this end, given $(s, \nabla, \psi) \in H_2$, we apply (2.7) and find that

$$A_\sigma((s, \nabla, \psi), (s, \nabla, \psi)) \geq \int_\Omega \partial(\sigma) s \cdot s + \kappa_1 \| \nabla s \|_{0, \Omega}^2 - \kappa_1 \| s \|_{0, \Omega} \| \nabla \|_{1, \Omega} + \kappa_2 \| \nabla \|_{0, \Omega} \| \nabla \|_{1, \Omega}^2 + \kappa_2 \| \nabla \|_{0, \Omega} \| \nabla \|_{1, \Omega}^2$$

$$+ \kappa_3 \| \nabla \|_{1, \Omega} - \kappa_3 \| s \|_{0, \Omega} \| \nabla \|_{1, \Omega} + \kappa_4 \| \nabla \|_{0, \Gamma}^2$$

$$\geq \theta_0 \| s \|_{0, \Omega}^2 + \kappa_1 \| \nabla \|_{0, \Omega}^2 + \kappa_2 \| \nabla \|_{0, \Omega}^2 - \frac{\kappa_1 \theta_2}{2\delta} \| s \|_{0, \Omega}^2 - \frac{\kappa_1 \theta_2}{2} \| \nabla \|_{0, \Omega}^2$$

$$+ \kappa_3 \| \nabla \|_{1, \Omega} - \frac{\kappa_3}{2\delta} \| s \|_{0, \Omega}^2 - \frac{\kappa_3}{2} \| \nabla \|_{1, \Omega} + \kappa_4 \| \nabla \|_{0, \Gamma}^2$$

$$= \left( \theta_0 - \frac{\kappa_1 \theta_2}{2 \delta} \right) \| s \|_{0, \Omega}^2 + \kappa_1 \left( 1 - \frac{\theta_2}{2 \delta} \right) \| \nabla \|_{0, \Omega}^2 + \kappa_2 \| \nabla \|_{0, \Omega}^2$$

$$+ \kappa_3 \left( 1 - \frac{\delta}{2} \right) \| \nabla \|_{1, \Omega}^2 + \kappa_4 \| \psi \|_{0, \Gamma}^2.$$

Then, assuming the stipulated hypotheses on $\delta, \bar{\delta}, \kappa_1, \kappa_2, \kappa_3, \kappa_4$ and applying Lemma 3.2, we can define

$$\tilde{\alpha}_1 := \left( \theta_0 - \frac{\kappa_1 \theta_2}{2 \delta} \right) - \frac{\kappa_3}{2\delta}, \quad \tilde{\alpha}_2 := \min \left\{ \kappa_1 \left( 1 - \frac{\theta_2}{2 \delta} \right), \kappa_2 \right\}, \quad \tilde{\alpha}_3 := \min \left\{ \kappa_3 \left( 1 - \frac{\delta}{2} \right), \kappa_4 \right\},$$

which allows us to deduce from (3.17) that

$$A_\sigma((s, \nabla, \psi), (s, \nabla, \psi)) \geq \tilde{\alpha} \| (s, \nabla, \psi) \|_{H_2}^2 \quad \forall (s, \nabla, \psi) \in H_2,$$

where $\tilde{\alpha} := \min(\tilde{\alpha}_1, \tilde{\alpha}_2, \tilde{\alpha}_3)$ is the ellipticity constant of $A_\sigma$. Next, applying Cauchy–Schwarz’s inequality, the trace estimates in $H(\text{div}; \Omega)$ and $H^1(\Omega)$, with constants $1$ and $c_0$, respectively, the upper bound for $g$ given in (2.5), and the fact that $\| \cdot \|_{l, r} \leq \| \cdot \|_{1, r}$ to (3.8), we find that

$$\| G_u(s, \nabla, \psi) \|_{l, r} = \| \nabla \cdot (\tau \cdot \phi, \phi) \|_{l, r} + \int_\Omega \psi \nabla g(u) - \kappa_2 \int_\Omega \nabla \nabla \nabla \nabla + \kappa_4 \int_{\Gamma} \phi_0 \psi \nabla \nabla$$

$$\leq \| \nabla \cdot (\tau \cdot \phi, \phi) \|_{1, r} + \| \nabla \nabla \nabla \nabla \|_{1, r} + \| \kappa_2 \nabla \nabla \nabla \nabla \|_{1, r} + \| \nabla \nabla \nabla \nabla \|_{1, r} + \| \kappa_4 \int_{\Gamma} \phi_0 \psi \|_{l, r},$$

which yields the existence of a positive constant $\| \hat{G} \|$, depending on $\kappa_2, \kappa_4$ and $c_0$, such that

$$\| G_u \|_{H_2} \leq \| \hat{G} \| \left\{ \| \phi_0 \|_{1, r} + \| g \|_{1, r} \right\}.$$

Finally, a direct application of the Lax–Milgram lemma proves that for each $(\sigma, u) \in H_0(\text{div}; \Omega) \times L^2(\Omega)$, problem (3.6) has a unique solution $S_{\sigma}(\sigma, u) = (\tau, \phi, \phi) \in H_2$. Moreover, a continuous dependence result is given by

$$\| S_{\sigma}(\sigma, u) \|_{H_2} = \| (\tau, \phi, \phi) \|_{H_2} = \frac{1}{\alpha} \| G_u \|_{H_2} \leq \tilde{c}_5 \| \phi_0 \|_{1, r} + \| g \|_{1, r},$$

where $\tilde{c}_5 := \frac{1}{\alpha}$, completing the proof. □

Note that the constants $\tilde{\alpha}_2$ and $\tilde{\alpha}_3$, being each one defined by the minimum between two quantities, can be maximized separately by making the corresponding quantities equal, that is by choosing $\kappa_2$ and $\kappa_4$ such that

$$\kappa_2 = \kappa_1 \left( 1 - \frac{\delta \theta_2}{2} \right) \quad \text{and} \quad \kappa_4 = \kappa_3 \left( 1 - \frac{\delta}{2} \right).$$

In turn, in order to guarantee that the rest of the constants involved are bounded away from zero, we take the parameters $\delta, \bar{\delta}, \kappa_1$, and $\kappa_3$ as the middle points of their feasible ranges. According to the above, we adopt the following choices:

$$\delta = \frac{1}{\theta_0}, \quad \kappa_1 = \frac{\delta \theta_0}{\theta_2} = \frac{\theta_0}{\theta_2}, \quad \bar{\delta} = 1, \quad \kappa_3 = \bar{\delta} \left( \theta_0 - \frac{\kappa_1 \theta_2}{2\delta} \right) = \frac{\theta_0}{2\delta},$$

$$\kappa_2 = \kappa_1 \left( 1 - \frac{\delta \theta_2}{2} \right) = \frac{\theta_0}{2\theta_2}, \quad \kappa_4 = \kappa_3 \left( 1 - \frac{\delta}{2} \right) = \frac{\theta_0}{4\delta},$$

which yield

$$\tilde{\alpha}_1 = \frac{\theta_0}{4}, \quad \tilde{\alpha}_2 = \frac{\theta_0}{2\theta_2}, \quad \tilde{\alpha}_3 = \frac{\theta_0}{4}, \quad \text{and} \quad \tilde{\alpha} = \min \left\{ \min \left\{ c_2, 1 \right\} \frac{\theta_0}{4}, \frac{\theta_0}{2\theta_2} \right\}.$$
We end this section by introducing suitable regularity estimates on $S$ and $\tilde{S}$, exactly as in [16, Section 2.2]. In fact, we concentrate in the case where $\Omega$ is a convex polygonal domain and $n = 2$, recall that $f(\psi) \in H^1(\Omega)$ for each $\psi \in H^1(\Omega)$, and assume from now on that $u_0 \in H^{3/2+\gamma}(\Gamma)$, where $\gamma$ is the positive constant whose existence is guaranteed in [27]. Then, applying precisely the estimate given in [27, eq. (3.9)] and recalling from the constitutive equation that the regularities of the unknowns are connected, we find that $S(\psi) \in H_0(\text{div}; \Omega) \cap H^{1/2}(\Omega) \times H^{\gamma/2}(\Omega) \cap L^2(\text{div}; \Omega) \cap H^{1/2+\gamma}(\Omega)$.

In turn, for $\tilde{S}$ we note that, for a given pair $(\zeta, w) := (S_1(\psi), S_2(\psi)) \in H_0(\text{div}; \Omega) \cap H^{1/2}(\Omega) \times H^{\gamma/2}(\Omega)$ (which denote the first and second components of the unique solution produced by the operator $S$), the hypothesis given by relation (2.8) implies in particular that $g(w) \in H^\gamma(\Omega)$. Additionally, we assume that the coefficients $\tilde{\theta}(\xi)$ are in $C^{1/2}(\bar{\Omega})$ and $\phi_0 \in H^{1/2+\gamma}(\Gamma)$, then elliptic regularity results (cf. [28, 29]) guarantee that $\phi := \tilde{S}_3(\zeta, w) \in H^{2+\gamma/2}(\Omega)$, and therefore there exists $\tilde{C}_1 > 0$ such that

$$\|\tilde{S}_3(\zeta, w)\|_{1,\gamma,\Omega} = \|\theta\|_{1,\gamma,\Omega} \leq \|\phi\|_{2,\gamma,\Omega} \leq \tilde{C}_1 \{\|\phi_0\|_{3/2+\gamma,\Gamma} + \|g(w)\|_{\gamma,\Omega}\}. \quad (3.21)$$

On the other hand, the Sobolev embedding theorem (cf. [30, Thm. A5]) establishes the continuous injection $i_\gamma : H^{1+\gamma}(\Omega) \longrightarrow C^0(\bar{\Omega})$, with boundedness constant $\tilde{C}_\gamma$. Then, applying (3.21) implies that

$$\|\tilde{S}_3(\zeta, w)\|_{\infty,\Omega} = \|\theta\|_{\infty,\Omega} \leq \tilde{C}_\gamma \|\phi\|_{1,\gamma,\Omega} \leq \tilde{C}_\gamma \tilde{C}_1 \{\|\phi_0\|_{3/2+\gamma,\Gamma} + \|g(w)\|_{\gamma,\Omega}\}. \quad (3.22)$$

Finally, replacing the estimates (2.8) and (3.14) into (3.22), we find that

$$\|\tilde{S}_3(\zeta, w)\|_{\infty,\Omega} = \|\theta\|_{\infty,\Omega} \leq C_\infty \{\|\phi_0\|_{3/2+\gamma,\Gamma} + \|u_0\|_{1/2,\gamma}\} + f_0\|\Omega|^{1/2}\}, \quad (3.23)$$

where $C_\infty$ is a positive constant depending on $C_\gamma$, $c_\gamma$, $\tilde{C}_\gamma$, $\tilde{C}_1$ (cf. (2.8), (3.14), (3.21), (3.22)).

### 3.3. Solvability analysis of the fixed-point equation

We now verify the hypotheses of the Schauder fixed-point theorem (see, e.g. [31, Theorem 9.12-1]). Before starting the result to be proved, we restrict $T$ to a ball and show that this operator maps into itself.

**Lemma 3.5.** Let $W$ be the closed and convex subset of $H^1(\Omega)$ defined by

$$W := \{\phi \in H^1(\Omega) : \|\phi\|_{1,\Omega} \leq \tilde{C}_5 \{\|u_0\|_{1/2,\Omega} + g_0\|\Omega|^{1/2}\}\},$$

where $\tilde{C}_5$ is the constant given by (3.14). Then $T(W) \subseteq W$.

**Proof.** It suffices to recall the definition of $T$ and apply the estimate (3.15). \(\square\)

The following estimate is key to derive Lipschitz continuity of $T$. For a proof see [16, Lemma 2.6].

**Lemma 3.6.** There exists a positive constant $C_\beta$ depending on $\mu$, $L_\gamma$, $\alpha$ (cf. (2.4), (3.12)) and the inf–sup constant of $b$, such that

$$\|S(\phi) - S(\psi)\|_{H^1} \leq C_\beta \|\phi - \psi\|_{0,\Omega}, \quad \forall \phi, \psi \in H^1(\Omega). \quad (3.24)$$

We are in a position to establish the announced property of the operator $T$.

**Lemma 3.7.** Let $C_\beta$ be the constant provided by Lemma 3.6. Then, for each $\phi, \psi \in H^1(\Omega)$, there holds

$$\|T(\phi) - T(\psi)\|_{1,\Omega} \leq \frac{C_\beta}{\alpha} \{L_\theta(1 + \kappa_2^2)^{1/2} + L_\phi(1 + \kappa_1^2)^{1/2}\|\tilde{S}_3(\zeta, w)\|_{\infty,\Omega}\} \|\phi - \psi\|_{0,\Omega}. \quad (3.25)$$

**Proof.** We begin by recalling that $T(\phi) = \tilde{S}_3(S_1(\phi), S_2(\phi))$ and $T(\psi) = \tilde{S}_3(S_1(\psi), S_2(\psi)) \forall \phi, \psi \in H^1(\Omega)$. For notational purposes we rename

$$(\sigma, u) := (S_1(\phi), S_2(\phi)) \quad \text{and} \quad (\zeta, w) := (S_1(\psi), S_2(\psi)).$$

where $(\sigma, u), (\zeta, w) \in H_0(\text{div}; \Omega) \times L^2(\Omega)$. Next, we consider $(t, \tilde{\sigma}, \phi) := \tilde{S}(\sigma, u)$ and $(r, \tilde{\zeta}, \psi) := \tilde{S}(\zeta, w)$, that is, for each $(\sigma, \tilde{\sigma}, \phi) \in H_2$, one has

$$A_\sigma((t, \tilde{\sigma}, \phi), (s, \tilde{\sigma}, \psi)) = G_u(s, \tilde{\sigma}, \psi) \quad \text{and} \quad A_\zeta(r, \tilde{\zeta}, \psi)(s, \tilde{\sigma}, \psi)) = G_w(s, \tilde{\sigma}, \psi).$$

Analogously to the proof of [16, Lemma 2.7], we apply the ellipticity of $A_\sigma$ (cf. (3.18)) and then, by adding and subtracting appropriate terms, we find that

$$\tilde{\alpha}\|((t, \tilde{\zeta}, \phi) - (r, \tilde{\zeta}, \phi))\|^2_{H_2} \leq A_\sigma((t, \tilde{\zeta}, \phi), (t, \tilde{\zeta}, \phi) - (r, \tilde{\zeta}, \phi)) - A_\sigma((r, \tilde{\zeta}, \phi), (t, \tilde{\zeta}, \phi) - (r, \tilde{\zeta}, \phi)) \quad \text{for each} \quad (s, \tilde{\sigma}, \psi) \in H_2. \quad (3.26)$$

$$= (G_u - G_w)((t, \tilde{\zeta}, \phi) - (r, \tilde{\zeta}, \phi)) + (A_\sigma - A_\zeta)((r, \tilde{\zeta}, \phi), (t, \tilde{\zeta}, \phi) - (r, \tilde{\zeta}, \phi)).$$
where the inequalities (3.26), (3.27) and (3.28) imply that
\[
\|(A_\sigma - A_0)(\tau, \tilde{\sigma}, \phi) - (r, \tilde{\tau}, \phi)\|_{H^2}\leq L_0 \|\sigma - \xi\|_{\Omega, \Omega} \left\{ \|\tau - r\|_{\Omega, \Omega} + \kappa_1 \|\tilde{\sigma} - \tilde{\xi}\|_{\Omega, \Omega} \right\}.
\]
whence the inequalities (3.26), (3.27) and (3.28) imply that
\[
\|(A_\sigma - A_0)(\tau, \tilde{\sigma}, \phi) - (r, \tilde{\tau}, \phi)\|_{H^2} \leq L_0 (1 + \kappa_1^2)^{1/2} \|\sigma - \xi\|_{\Omega, \Omega} \left\{ \|\tau - r\|_{\Omega, \Omega} + \kappa_1 \|\tilde{\sigma} - \tilde{\xi}\|_{\Omega, \Omega} \right\}.
\]
Next, according to the definitions given when starting the proof, we can rewrite (3.29) as
\[
\|\tilde{S}(S_1(\phi), S_2(\phi)) - \tilde{S}(S_1(\phi), S_2(\phi))\|_{H^2} = \frac{1}{\alpha} \left\{ L_0 (1 + \kappa_1^2)^{1/2} \|\sigma - \xi\|_{\Omega, \Omega} \left\{ \|\tau - r\|_{\Omega, \Omega} + \kappa_1 \|\tilde{\sigma} - \tilde{\xi}\|_{\Omega, \Omega} \right\} \right\}.
\]
It is important to note here that, when needed, \(\|\tilde{S}(S_1(\phi), S_2(\phi))\|_{\Omega, \Omega}\) can be bounded by (3.23), for each \(\phi \in H^1(\Omega)\). Finally, applying estimates (3.24) and (3.30), we find that
\[
\|T(\phi) - T(\psi)\|_{1, \Omega, \Omega} = \|\tilde{S}(S_1(\phi), S_2(\phi)) - \tilde{S}(S_1(\phi), S_2(\phi))\|_{1, \Omega, \Omega} \leq \frac{1}{\alpha} \left\{ |S_1(\phi), S_2(\phi)|_{\Omega, \Omega} \left\{ \|\tau - r\|_{\Omega, \Omega} + \kappa_1 \|\tilde{\sigma} - \tilde{\xi}\|_{\Omega, \Omega} \right\} \right\}.
\]
which gives (3.25), completing the proof. □

The next lemma establishes the continuity and compactness of \(T\).

**Lemma 3.8.** Let \(W\) be as in **Lemma 3.5**. Then \(T : W \to W\) is continuous and \(\overline{T(W)}\) is compact.

**Proof.** It follows straightforwardly from (3.25) and the continuity of \(i_k : H^1(\Omega) \to L^2(\Omega)\) that
\[
\|T(\phi) - T(\psi)\|_{1, \Omega} \leq \frac{1}{\alpha} |S_1(\phi), S_2(\phi)|_{\Omega, \Omega} \left\{ \|\tau - r\|_{\Omega, \Omega} + \kappa_1 \|\tilde{\sigma} - \tilde{\xi}\|_{\Omega, \Omega} \right\} \|\phi - \psi\|_{1, \Omega},
\]
which proves continuity of \(T\). In turn, let \(\{\phi_k\}_{k \in \mathbb{N}}\) be a sequence of \(W\), which is clearly bounded. Then, there exists a subsequence \(\{\phi_k^{(i)}\}_{k \in \mathbb{N}} \subseteq \{\phi_k\}_{k \in \mathbb{N}}\) such that \(\phi_k^{(i)} \rightharpoonup \phi \in H^1(\Omega)\). In this way, thanks to the compactness of \(i_k\), we deduce that \(\phi_k^{(i)} \to \phi \in L^2(\Omega)\), which, combined with (3.25), implies that \(T(\phi_k^{(i)}) \to T(\phi) \in H^1(\Omega)\), and proves the compactness of \(\overline{T(W)}\). □

We are ready now to prove that (3.10) is well-posed. From **Lemmas 3.5** and 3.8, the existence of solution is merely an application of Schauder’s theorem. Furthermore, assuming that the data is small enough, we can prove uniqueness of solution. This is indeed possible thanks to the regularity estimates established at the end of Section 3.2.

Details of the proof are similar to those available in [16, Thm. 2.9].

**Theorem 3.9.** Let \(W\) be as in **Lemma 3.5**. Then, the augmented fully-mixed problem (3.9) has at least one solution \((\sigma, (\mathbf{u}, \rho)) = (\mathbf{u}, \tilde{\sigma}, \phi) \in H_1 \times H_2\) with \(\phi \in W\), satisfying the bounds
\[
\|\mathbf{u}\|_{1, \Omega, \Omega} \leq C_0 \|\phi_0\|_{1/2, r}^2 + C_2 |\Omega|^{1/2},
\]
\[
\|\sigma\|_{H_1} \leq C_0 \|\mathbf{u}_0\|_{1/2, r}^2 + C_2 |\Omega|^{1/2}.
\]
Moreover, if the data satisfy
\[
\frac{1}{\alpha} C_0 \left\{ |\mathbf{u}_0|_{1/2, r}^2 + C_2 |\Omega|^{1/2} \right\} < 1,
\]
then the solution \(\phi\) is unique in \(W\).
4. The Galerkin scheme and well-posedness of the discrete problem

In this section we introduce and analyse a Galerkin scheme for (3.9). We adopt the discrete analogue of the fixed-point strategy introduced in Section 3.2 and apply the Brouwer fixed-point theorem to prove existence of discrete solution. We start by considering generic finite dimensional subspaces
\[ H_h^s \subseteq H_0^s(\Omega), \quad H_h^p \subseteq L^2(\Omega), \quad \mathbb{I}_h^p \subseteq \mathbb{I}_h^2(\Omega), \quad (4.1) \]
\[ H_h^1 \subseteq L^2(\Omega), \quad H_h^0 \subseteq H(div; \Omega), \quad \text{and} \quad H_h^0 \subseteq H^1(\Omega), \quad (4.2) \]
which will be specified later on. Hereafter, \( h \) denotes the size of a regular partition \( \mathcal{T}_h \) of \( \Omega \) into triangles \( K \) of diameter \( h_k \), i.e. \( h := \max \{ h_k : K \in \mathcal{T}_h \} \). A Galerkin scheme for (3.9) reads: find \((\sigma_h, (u_h, \rho_h), t_h, \phi_h) \in H_h^s \times (H_h^1 \times H_h^0) \times H_h^1 \times H_h^0\) such that
\[
ap(\sigma_h, \tau_h) + b(\tau_h, (u_h, \rho_h)) = G(\tau_h) \quad \forall \tau_h \in H_h^s, \\
b(\sigma_h, (v_h, \eta_h)) = F_{\phi h}(v_h, \eta_h) \quad \forall (v_h, \eta_h) \in H_h^u \times H_h^p, \\
A_{\phi h}((t_h, \phi_h), (s_h, \tau_h, \psi_h)) = G_{u h}(s_h, \tau_h, \psi_h) \quad \forall (s_h, \tau_h, \psi_h) \in H_h^s \times H_h^2 \times H_h^0. \tag{4.3} \]

In order to address the well-posedness of (4.3), we proceed analogously as in Section 3.2 and apply a fixed-point strategy. In fact, we define the operator \( S_h : H_h^s \to \mathbb{I}_h^p \times (H_h^1 \times H_h^0) \) as
\[
S_h(\phi_h) := (S_{1,h}(\phi_h), (S_{2,h}(\phi_h), S_{3,h}(\phi_h))) := (\sigma_h, (u_h, \rho_h)) \quad \forall \phi_h \in H_h^o,
\]
where \((\sigma_h, (u_h, \rho_h))\) is the unique solution of\n\[
ap(\sigma_h, \tau_h) + b(\tau_h, (u_h, \rho_h)) = G(\tau_h) \quad \forall \tau_h \in H_h^s, \\
b(\sigma_h, (v_h, \eta_h)) = F_{\phi h}(v_h, \eta_h) \quad \forall (v_h, \eta_h) \in H_h^u \times H_h^p, \tag{4.4} \]
with \( F_{\phi h} \) being defined by (3.2) with \( \phi = \phi h \). In turn, we introduce \( \tilde{S}_h : \mathbb{I}_h^p \times H_h^1 \to H_h^1 \times H_h^2 \times H_h^p \) as
\[
\tilde{S}_h(\sigma_h, u_h) := (\tilde{S}_{1,h}(\sigma_h, u_h), \tilde{S}_{2,h}(\sigma_h, u_h), \tilde{S}_{3,h}(\sigma_h, u_h)) := (t_h, \phi h, \tau_h) \quad \forall (\sigma_h, u_h) \in \mathbb{I}_h^p \times H_h^1, \tag{4.5} \]
where \((t_h, \phi h, \tau_h)\) is the unique solution of
\[
A_{\phi h}((t_h, \phi h, \tau_h), (s_h, \tau_h, \psi h)) = G_{u h}(s_h, \tau_h, \psi h) \quad \forall (s_h, \tau_h, \psi h) \in H_h^s \times H_h^2 \times H_h^p.
\]

Analogously to the continuous case, we first study the well-posedness of \( S_h \) and \( \tilde{S}_h \), and hence the well-definiteness of \( T_h \). To this end we proceed as in [16, Section 3.2] and incorporate further hypotheses on the discrete spaces \( \mathbb{I}_h^s, H_h^u \) and \( H_h^p \). Let \( V_h \) be the discrete kernel of \( b \) given by
\[
V_h := \{ \tau_h \in H_h^p : b(\tau_h, (v_h, \eta_h)) = 0 \quad \forall (v_h, \eta_h) \in H_h^u \times \mathbb{I}_h^p \},
\]
and assume the following discrete inf–sup conditions:

(H.0) There exists a constant \( \alpha_1 > 0 \), independent of \( h \), such that
\[
\sup_{\|\tau_h\|_{\mathbb{I}_h^p} \neq 0} \frac{a(\sigma_h, \tau_h)}{\|\tau_h\|_{\mathbb{I}_h^p}} \geq \alpha_1 \|\sigma_h\|_{div; \Omega} \quad \forall \sigma_h \in V_h. \tag{4.7} \]

(H.1) There exists a constant \( \beta_1 > 0 \), independent of \( h \), such that
\[
\sup_{\|\tau_h\|_{\mathbb{I}_h^p} \neq 0} \frac{b(\tau_h, (v_h, \eta_h))}{\|\tau_h\|_{\mathbb{I}_h^p}} \geq \beta_1 \|(v_h, \eta_h)\|_{L^2(\Omega) \times \mathbb{I}_h^p(\Omega)} \quad \forall (v_h, \eta_h) \in H_h^u \times H_h^p. \tag{4.8} \]

Deriving well-posedness of the discrete problem (4.4) results as a straightforward application of the discrete Babuška–Brezzi theory. Firstly, the operators related to \( a \) and \( b \), and the functionals \( G \) and \( F_{\phi h} \) are all bounded on subspaces of the
corresponding continuous spaces. Next, the inf–sup conditions are given by (H.0) and (H.1). The unique solvability of (4.4) is abridged in the following lemma.

Lemma 4.1. For each , problem (4.4) has a unique solution \( \mathbf{S}_h(\phi_h) := (\sigma_h, (u_h, \rho_h)) \in \mathbb{H}_h^\sigma \times (\mathbb{H}_h^u \times \mathbb{H}_h^\rho) \). Moreover, there exists \( C > 0 \), depending on \( \mu, \alpha_1 \), and \( \beta_1 \) (cf. (4.7), (4.8)), but independent of \( \phi_h \) and \( h \), such that

\[
\| \mathbf{S}_h(\phi_h) \|_{\mathbf{H}_h} = \left\| (\sigma_h, (u_h, \rho_h)) \right\|_{\mathbf{H}_h} \leq C \left( \| u_0 \|_{1/2, r} + f_2 |\Omega|^{1/2} \right).
\]

In regard to the problem defined by \( \tilde{\mathbf{S}}_h \), we state next the discrete analogue of Lemma 3.4.

Lemma 4.2. Assume that \( \kappa_1 \in \left( 0, \frac{2\delta_0}{\sigma_0} \right) \) and \( \kappa_3 \in \left( 0, 2 \tilde{\gamma} \left( \phi_0 - \frac{\kappa_2}{2} \right) \right) \) with \( \delta_0 = \left( 0, \frac{\beta_1}{\sigma_2} \right) \), \( \tilde{\gamma} = (0, 2) \), and \( \kappa_2, \kappa_4 > 0 \). Then, for each \( (\sigma_h, u_h) \in \mathbb{H}_h^\sigma \times \mathbb{H}_h^u \), problem (4.5) has a unique solution \( \tilde{\mathbf{S}}_h(\sigma_h, u_h) = (t_h, \tilde{\sigma}_h, \tilde{\phi}_h) \in \tilde{\mathbb{H}}_h^\sigma \times \tilde{\mathbb{H}}_h^\sigma \times \tilde{\mathbb{H}}_h^\rho \). Moreover, with the constant \( C_S \) provided by Lemma 3.4, there holds

\[
\| \tilde{\mathbf{S}}_h(\sigma_h, u_h) \|_{\mathbf{H}_h} = \left\| (t_h, \tilde{\sigma}_h, \tilde{\phi}_h) \right\|_{\mathbf{H}_h} \leq C \left\| \phi_0 \|_{1/2, r} + g_2 |\Omega|^{1/2} \right\|.
\]

Proof. We first observe that for each \( (\sigma_h, u_h) \in \mathbb{H}_h^\sigma \times \mathbb{H}_h^u \), the operator \( \mathbb{A}_{\sigma_h} \) is bounded and elliptic on \( \mathbb{H}_h^\sigma \times \tilde{\mathbb{H}}_h^\sigma \times \tilde{\mathbb{H}}_h^\rho \) with the same constants \( \| A \| \) and \( \tilde{\alpha} \) from Lemma 3.4. In addition, \( \tilde{\gamma}_{\sigma_h} \) restricted to \( \mathbb{H}_h^\sigma \times \tilde{\mathbb{H}}_h^\sigma \times \tilde{\mathbb{H}}_h^\rho \) is bounded as in (3.19) with \( u_h \) in place of \( u \). Therefore, the result is a direct application of the Lax–Milgram lemma. \( \square \)

We notice in advance that, instead of the regularity estimates employed in the continuous case (not applicable in the present discrete case), we simply utilize properties of the discrete subspaces chosen. In what follows, we verify the hypotheses of the Brouwer fixed-point theorem (see, e.g., [31, Thm. 9.9-2]) to prove that \( T_h \) has at least one fixed point.

Lemma 4.3. Let \( W_h := \left\{ \phi_h \in \mathbb{H}_h^\phi : \| \phi_h \|_{1, \Omega} \leq C \left( \| \phi_0 \|_{1/2, r} + g_2 |\Omega|^{1/2} \right) \right\} \). Then \( T_h(W_h) \subseteq W_h \).

Proof. It is basically an application of the definition of \( T_h \) and the estimate (4.9). \( \square \)

Lemma 4.4. There exists \( C > 0 \) depending on \( \mu, L_f, \alpha_1 \), and \( \beta_1 \) (cf. (2.4), (4.7), (4.8)) such that

\[
\| \mathbf{S}_h(\phi_h) - \mathbf{S}_h(\psi_h) \|_{\mathbf{H}_h} \leq C \| \phi_h - \psi_h \|_{0, \Omega} \quad \forall \phi_h, \psi_h \in \mathbb{H}_h^\phi.
\]

Proof. See [16, Lemma 3.4]. \( \square \)

Lemma 4.5. For each \( (\sigma_h, u_h), (\zeta_h, w_h) \in \mathbb{H}_h^\sigma \times \mathbb{H}_h^u \), there holds

\[
\| \tilde{\mathbf{S}}_h(\sigma_h, u_h) - \tilde{\mathbf{S}}_h(\zeta_h, w_h) \|_{\mathbf{H}_h} \leq \frac{1}{\tilde{\alpha}} \left( L_g(1 + \kappa_2^2)^{1/2} \| u_h - w_h \|_{0, \Omega} + L_f(1 + \kappa_2^2)^{1/2} \| \tilde{\mathbf{S}}_h(\sigma_h, u_h) \|_{\infty, \Omega} \| \sigma_h - \zeta_h \|_{0, \Omega} \right).
\]

Proof. Proceeding as in [16, Lemma 3.5], given \( (\sigma_h, u_h), (\zeta_h, w_h) \in \mathbb{H}_h^\sigma \times \mathbb{H}_h^u \), we let \( (t_h, \tilde{\sigma}_h, \tilde{\phi}_h) = \tilde{\mathbf{S}}_h(\sigma_h, u_h) \) and \( (r_h, \tilde{\zeta}_h, \phi_h) = \tilde{\mathbf{S}}_h(\zeta_h, w_h) \). Then, analogously to the proof of Lemma 3.7, we get

\[
\| \tilde{\alpha} \| \| t_h - \tilde{\sigma}_h, \phi_h \|_{\mathbf{H}_h} \leq \left( L_g(1 + \kappa_2^2)^{1/2} \| u_h - w_h \|_{0, \Omega} + L_f(1 + \kappa_2^2)^{1/2} \| r_h \|_{\infty, \Omega} \| \sigma_h - \zeta_h \|_{0, \Omega} \right) \| \phi_h - \phi_h \|_{0, \Omega}.
\]

Since the elements of \( \mathbb{H}_h^u \) are piecewise polynomials (to be specified later on) it follows that \( \| r_h \|_{\infty, \Omega} < +\infty \), and hence the foregoing equation yields (4.10). Further details are omitted. \( \square \)

As a consequence of the above Lemmas, we can state the Lipschitz continuity of \( T_h \).

Lemma 4.6. Assume that \( C \) is as in Lemma 4.4. Then, for each \( \phi_h, \psi_h \in \mathbb{H}_h^\phi \), there holds

\[
\| T_h(\phi_h) - T_h(\psi_h) \|_{1, \Omega} \leq C \frac{1}{\tilde{\alpha}} \left( L_g(1 + \kappa_2^2)^{1/2} + L_f(1 + \kappa_2^2)^{1/2} \| \tilde{\mathbf{S}}_h(\sigma_h, u_h) \|_{\infty, \Omega} \right) \| \phi_h - \psi_h \|_{0, \Omega}.
\]

Proof. It suffices to recall that \( T_h(\phi_h) = \tilde{\mathbf{S}}_h(\mathbf{S}_h(\phi_h), \phi_h) \) for \( \phi_h \in \mathbb{H}_h^\phi \) and apply Lemmas 4.4 and 4.5. \( \square \)
At this point, we are able to state the main result of this section.

**Theorem 4.7.** Let $W_h := \{ \phi_h \in H^2_h : \| \phi_h \|_{1,\Omega} \leq C_{h} (\| \phi_D \|_{1/2,\tau} + g_2|\Omega|^{1/2}) \}$. Then (4.3) has at least one solution $(\sigma_h, (u_h, \rho_h), t_h, \tilde{\sigma}_h, \phi_h) \in H^2_h \times (H^2_h \times H^2_h) \times H^2_h \times H^2_h$ with $\phi_h \in W_h$, and there holds

\[ \| (t_h, \tilde{\sigma}_h, \phi_h) \|_{H^2} \leq C_h (\| \phi_D \|_{1/2,\tau} + g_2|\Omega|^{1/2}) , \]

\[ \| (\sigma_h, (u_h, \rho_h)) \|_{H^2} \leq C_h (\| u_D \|_{1/2,\tau} + f_2|\Omega|^{1/2}) . \tag{4.11} \]

\[ \| (\sigma_h, (u_h, \rho_h), t_h, \tilde{\sigma}_h, \phi_h) \| \] for which, we suggest to estimate $\| (\sigma, (u, \rho)) \|_H$ and $\| (\sigma, (u, \rho)) \|_H$, separately. With this goal in mind, we first rearrange (3.9) and (4.3) as follows

\[ a(\sigma, \tau) + b(\tau, (u, \rho)) = G(\tau), \quad \forall \tau \in \mathbb{H}_0^h(\text{div}; \Omega), \]

\[ b(a, \sigma, \tau) + b(v, (u, \rho)) = F(a, \sigma, \tau), \quad \forall \sigma, v \in \mathbb{H}_0^h, \]

\[ a(\sigma, \tau) + b(\tau, (u, \rho)) = G(\tau), \quad \forall \tau \in \mathbb{H}_0^h, \]

\[ b(a, \sigma, \tau) + b(v, (u, \rho)) = F(a, \sigma, \tau), \quad \forall \sigma, v \in \mathbb{H}_0^h. \tag{5.1} \]

Next, we recall from [32, Thm. 11.2 and 11.1] two instrumental results. First, a Strang inequality for saddle point problems where continuous and discrete formulations differ only in the functional. This will be applied to (5.1). Second, the standard Strang Lemma for elliptic problems, which fits (5.2). We will not write them explicitly here but will refer to these lemmas as Saddle-point Strang Lemma, and Elliptic Strang Lemma, respectively.

From now on, we denote as usual

\[ \text{dist} ((\sigma, (u, \rho)), H^2_h \times (H^2_h \times H^2_h)) := \inf_{(\tau_h, (v, \eta)) \in (H^2_h \times (H^2_h \times H^2_h))} \| (\sigma, (u, \rho) - (\tau_h, (v, \eta)) \|_{H^2} , \]

and

\[ \| (t, \tilde{\sigma}, \phi, (s, \tilde{\sigma}, \psi)) \|_{H^2} = \| (u, \rho) - (s, \tilde{\sigma}, \psi) \|_{H^2}. \tag{5.2} \]

Next, a straightforward application of the Saddle-point Strang Lemma yields the following result concerning a priori estimates for $\| (\sigma, (u, \rho)) \|_H$ and $\| (\sigma, (u, \rho)) \|_H$. Details of the proof can be found in [16, Lemma 3.10].

**Lemma 5.1.** There exists a constant $C_{ST} > 0$, depending on $\mu$, $\alpha_1$ and $\beta_1$ (cf. (4.7), (4.8)), such that

\[ \| (\sigma, (u, \rho)) - (\sigma_h, (u_h, \rho_h)) \|_{H^2} \]

\[ \leq C_{ST} \left( \text{dist} ((\sigma, (u, \rho)), H^2_h \times (H^2_h \times H^2_h)) + \| \phi - \phi_h \|_{0,\Omega} \right) . \tag{5.3} \]

In turn, an estimate for $\| (t, \tilde{\sigma}, \phi) - (t_h, \tilde{\sigma}_h, \phi_h) \|_{H^2}$ reads as follows.

**Lemma 5.2.** Let $C_{ST} := \tilde{\alpha}^{-1} \max(1, \| A \|)$, where $\| A \|$ and $\tilde{\alpha}$ are the boundedness and ellipticity constants, respectively, of the bilinear form $A_h$ (cf. (3.16), (3.18)). Then, there holds

\[ \| (t, \tilde{\sigma}, \phi) - (t_h, \tilde{\sigma}_h, \phi_h) \|_{H^2} \]

\[ \| (u, \rho) - (u_h, \rho_h) \|_{0,\Omega} + L_\rho (1 + \kappa^2)^{1/2} \| (\sigma - \sigma_h) \|_{0,\Omega} \| \phi \|_{\infty,\Omega} \] . \tag{5.4}
Proof. Applying the elliptic Strang Lemma in the context of (5.2), gives
\[ \|(t, \tilde{\sigma}, \phi) - (t_h, \tilde{\sigma}_h, \phi_h)\|_{H^1} \]
\[ \leq \overline{C}_{ST} \left\{ \sup_{(r_h, \tilde{\zeta}_h, \phi_h) \in H^1_0} \frac{|G_u(r_h, \tilde{\zeta}_h, \phi_h) - G_{u_h}(r_h, \tilde{\zeta}_h, \phi_h)|}{\|r_h, \tilde{\zeta}_h, \phi_h\|} + \inf_{(s_h, \tilde{\zeta}_h, \phi_h) \in H^1_0} \left\{ \|(t, \tilde{\sigma}, \phi) - (s_h, \tilde{\zeta}_h, \phi_h)\| \right\} \right. \\
\[ \left. + \sup_{(r_h, \tilde{\zeta}_h, \phi_h) \in H^1_0} \frac{|A_u((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h)) - A_{u_h}((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h))|}{\|r_h, \tilde{\zeta}_h, \phi_h\|} \right\} \right\} \\
(5.5) \]
Then, proceeding analogously as in the proof of Lemma 3.7, we deduce that
\[ \sup_{(r_h, \tilde{\zeta}_h, \phi_h) \in H^1_0} \frac{|G_u(r_h, \tilde{\zeta}_h, \phi_h) - G_{u_h}(r_h, \tilde{\zeta}_h, \phi_h)|}{\|r_h, \tilde{\zeta}_h, \phi_h\|} \leq L_0(1 + \kappa_1^2)^{1/2} \|u - u_h\|_{0, \Omega}. \] \(5.6\)
In turn, in much the same way as [33, Lemma 5.2], we add and subtract suitable terms to write
\[ A_u((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h)) - A_{u_h}((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h)) \]
\[ = A_u((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h)) - (t, \tilde{\sigma}, \phi) + (A_u - A_{u_h})((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h)) \]
\[ + A_{u_h}((t, \tilde{\sigma}, \phi) - (s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h)). \]
thus, the estimates for the first and third terms follow by applying the boundedness (3.16), whereas for the second one, we find that
\[ (A_u - A_{u_h})(t, \tilde{\sigma}, \phi, (r_h, \tilde{\zeta}_h, \phi_h)) = \int_{\Omega} (\dot{\vartheta}(\sigma) - \dot{\vartheta}(\sigma_h)) t \cdot (r_h - \kappa_1 \tilde{\zeta}_h) \]
\[ \leq L_0(1 + \kappa_1^2)^{1/2} \|\sigma - \sigma_h\|_{0, \Omega} \|t\|_{0, \Omega} \|r_h, \tilde{\zeta}_h, \phi_h\|. \]
whence, we deduce that
\[ \sup_{(r_h, \tilde{\zeta}_h, \phi_h) \in H^1_0} \frac{|A_u((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h)) - A_{u_h}((s_h, \tilde{\zeta}_h, \phi_h), (r_h, \tilde{\zeta}_h, \phi_h))|}{\|r_h, \tilde{\zeta}_h, \phi_h\|} \]
\[ \leq 2 \|A\| \|(t, \tilde{\sigma}, \phi) - (s_h, \tilde{\zeta}_h, \phi_h)\| + L_0(1 + \kappa_1^2)^{1/2} \|\sigma - \sigma_h\|_{0, \Omega} \|t\|_{0, \Omega}. \] \(5.7\)
Finally, by replacing (5.6)–(5.7) into (5.5), we get (5.4), which ends the proof. \(\square\)
Now, to derive the Céa estimate for the total error we combine Lemmas 5.1 and 5.2. To this end, and for notational convenience, we introduce the following constants
\[ C_1 := C_{ST} \overline{C}_{ST} L_0(1 + \kappa_2)^{1/2}, \quad C_2 := C_{ST} \overline{C}_{ST} C_{\infty} L_0(1 + \kappa_1^2)^{1/2}, \quad C_3 := \overline{C}_{ST}(1 + 2 \|A\|). \]
Next we replace the bounds for \(\|u - u_h\|_{0, \Omega}\) and \(\|\sigma - \sigma_h\|_{0, \Omega}\) into (5.4), and apply from (3.23) that
\[ \|t\|_{0, \Omega} \leq C_{\infty} \left\{ \|\phi_0\|_{3/2 + \gamma, \Omega} + \|u_0\|_{1/2, \Omega} + f_2 |\Omega|^{1/2} \right\}. \]
We then perform algebraic manipulations to find that
\[ \|(t, \tilde{\sigma}, \phi) - (t_h, \tilde{\sigma}_h, \phi_h)\|_{H^1} \]
\[ \leq \left\{ C_1 + C_2 \left( \|\phi_0\|_{3/2 + \gamma, \Omega} + \|u_0\|_{1/2, \Omega} + f_2 |\Omega|^{1/2} \right) \right\} \text{dist} (\sigma, (u, \rho), H^r \times (H^r_h \times H^r_h)) \]
\[ + L_0 \left\{ C_1 + C_2 \left( \|\phi_0\|_{3/2 + \gamma, \Omega} + \|u_0\|_{1/2, \Omega} + f_2 |\Omega|^{1/2} \right) \right\} \|(t, \tilde{\sigma}, \phi) - (t_h, \tilde{\sigma}_h, \phi_h)\| \]
\[ + C_3 \left( (t, \tilde{\sigma}, \phi), H^r_h \times H^r_h \times H^r_h \right) \]
(5.8)
Consequently, we can establish the following result which provides the complete Céa estimate.

**Theorem 5.3.** Suppose that the data satisfy

\[ L_f \{ C_1 + C_2 (\| \phi_D \|_{3+2r} + \| u_D \|_{1+2r} + f_2 \| \Omega \|^{1/2}) \leq \frac{1}{2}, \]

Then, there exist positive constants \( C_4 \) and \( C_5 \) independent of \( h \), such that

\[
\| (\sigma, (u, \rho)) - (\sigma_h, (u_h, \rho_h)) \|_{H_1} + \| (t, \tilde{\sigma}, \phi) - (t_h, \tilde{\sigma}_h, \phi_h) \|_{H_2} \\
\leq C_4 \text{dist} ((\sigma, (u, \rho)), H^H \times H^H_j) + C_5 \text{dist} ((t, \tilde{\sigma}, \phi), H^H_\sigma \times H^H_\sigma + H^H_\sigma) .
\]

(5.9)

**Proof.** It follows straightforwardly from (5.3) and (5.8). \( \square \)

We now specify finite element subspaces satisfying (4.1)–(4.2) and the discrete inf–sup conditions (H.0)–(H.1). Given an integer \( k \geq 0 \), for each \( K \in \mathcal{T}_h \) we let \( P_k(K) \) be the space of polynomial functions on \( K \) of degree \( \leq k \) and define the local Raviart–Thomas space of order \( k \) as

\[ RT_k(K) := P_k(K) \oplus P_k(K) \times \]

where \( P_k(K) = [P_0(K)]^2 \), and \( x \) is the generic vector in \( \mathbb{R}^2 \). Let \( b_k \) be the element bubble function defined as the unique polynomial in \( P_{k+1}(K) \) vanishing on \( \partial K \) with \( \int_K b_k = 1 \). Then, for each \( K \in \mathcal{T}_h \) we consider the bubble space of order \( k \), defined by

\[ B_k(K) := P_k(K) \left( \frac{\partial b_k}{\partial x_2}, -\frac{\partial b_k}{\partial x_1} \right) . \]

One option to approximate stress, displacement and rotation is the classical PEERS elements [34]:

\[
H^\sigma_h := \{ \tau_h \in H_0(\text{div}; \Omega) : \tau_h |_{K} \in RT_k(K) \oplus B_k(K) \quad \forall K \in \mathcal{T}_h \}, \\
H^u_h := \{ v_h \in L^2(\Omega) : v_h |_{K} \in P_k(K) \quad \forall K \in \mathcal{T}_h \}, \\
H^\phi_h := \{ \eta_h \in L^2(\Omega) : \eta_h |_{K} \in C_k(\Omega) \quad \forall K \in \mathcal{T}_h \} .
\]

(5.10)

We could also employ the Arnold–Falk–Winther (AFW, [25]) elements for the elasticity unknowns:

\[
H^\sigma_h := \{ \tau_h \in H_0(\text{div}; \Omega) : \tau_h |_{K} \in BDM_k(K) \quad \forall K \in \mathcal{T}_h \}, \\
H^u_h := \{ v_h \in L^2(\Omega) : v_h |_{K} \in P_k(K) \quad \forall K \in \mathcal{T}_h \}, \\
H^\phi_h := \{ \eta_h \in L^2(\Omega) : \eta_h |_{K} \in P_k(K) \quad \forall K \in \mathcal{T}_h \} .
\]

(5.11)

and recall that both PEERS and AFW satisfy (H.0) and (H.1) (cf. [34, Lemma 4.4], [35, Thm. 11.9]).

In turn, we define the approximating spaces for the concentration gradient, diffusive flux and solute concentration as piecewise polynomials of degree \( \leq k \), Raviart–Thomas elements of order \( k \), and Lagrange finite elements up to degree \( k+1 \), respectively:

\[
H^\tau_h := \{ \tau_h \in L^2(\Omega) : \tau_h |_{K} \in P_k(K) \quad \forall K \in \mathcal{T}_h \}, \\
H^\phi_h := \{ \phi_h \in C(\Omega) : \phi_h |_{K} \in P_{k+1}(K) \quad \forall K \in \mathcal{T}_h \} .
\]

(5.12)

Approximation properties of the spaces in (5.10), (5.11), (5.12) can be found in e.g. [23,24]. They can be combined with the Céa estimate (5.9) and the assumption of adequately small data, to produce the theoretical rates of convergence of (4.3), summarized in what follows.

**Theorem 5.4.** In addition to the hypotheses of Theorems 3.9, 4.7 and 5.3, assume that there exists \( s > 0 \) such that \( \sigma \in H^s(\Omega) \), \( \text{div} \sigma \in H^{s-1}(\Omega) \), \( u \in H^s(\Omega) \), \( \rho \in H^s(\Omega) \), \( t \in H^s(\Omega) \), \( \tilde{\sigma} \in H^s(\Omega) \), \( \text{div} \tilde{\sigma} \in H^{s+\gamma}(\Omega) \) and \( \phi \in H^{s+\gamma}(\Omega) \). Then, there exists \( \widetilde{C} > 0 \), independent of \( h \), such that, with the finite element subspaces defined by either (5.10) or (5.11) and (5.12), there holds

\[
\text{min} \left\{ \left\| (\sigma, (u, \rho)) - (\sigma_h, (u_h, \rho_h)) \right\|_{H_1} + \left\| (t, \tilde{\sigma}, \phi) - (t_h, \tilde{\sigma}_h, \phi_h) \right\|_{H_2} \right\} \leq \widetilde{C}h^{\text{min}(s,k+1)} \left\{ \| \sigma \|_{s+\gamma} \right\} .
\]

(5.13)
6. Numerical results

In this section we present some examples illustrating the performance of our augmented fully-mixed scheme (4.3), and confirming the rates of convergence provided by Theorem 5.4. These numerical results also include examples in which some of the data do not necessarily satisfy all the hypotheses required, thus confirming the potentiality of the method proposed, and also evidencing that only technical limitations are preventing us from extending our theoretical analysis to more general cases. Our implementation is based on the Fenics library [36]. In turn, a Picard algorithm with tolerance of $10^{-5}$ on the $L^2$-norm of the residual has been employed for the fixed-point problem (4.6). The boundary conditions employed in Examples 2 and 3 were motivated by the specific application of stress-assisted diffusion problems in lithium batteries, and they correspond to mixed boundary conditions, which are currently not supported by our theoretical analysis. Nevertheless, the obtained results still show stable and robust computations, which insinuates that only technical difficulties prevent us of extending our analysis to the case of mixed boundary conditions. For the diffusion sub-problem in Example 2 we have utilized the variational formulation (3.4) applying a fixed-point on $\sigma$ and $t$; and $\sigma$ and $\phi$, respectively.

Example 1. In our first numerical test we take the unit square as computational domain $\Omega = (0, 1)^2$ and choose the following manufactured exact solutions and coupling terms to (3.9):

$$
\begin{align*}
\mathbf{u} &= \left( 
\begin{array}{c}
d_1 \cos(\pi x_1) \sin(\pi x_2) + \frac{x_2^2(1-x_2)^2}{2\lambda} \\
-d_1 \sin(\pi x_1) \cos(\pi x_2) + \frac{x_2^3(1-x_2)^3}{2\lambda}
\end{array}
\right), \quad
\sigma = \lambda \text{tr} \mathbf{e}(\mathbf{u}) I + 2\mu \mathbf{e}(\mathbf{u}), \quad
\rho = \nabla \mathbf{e}(\mathbf{u}),
\end{align*}
$$

(6.1)

We note that the tensorial diffusivity, body load and diffusive source terms satisfy (2.4)–(2.6) and (2.7). Moreover, the elasticity and diffusion equations are considered non-homogeneous and the extra source terms, as well as the non-homogeneous boundary data $u_0$ and $\phi_0$, are chosen according to (6.1). This treatment does not compromise the continuous and discrete analysis, as the smoothness of the exact solution provides right-hand sides with terms in $L^2(\Omega)$, thus only requiring a slight modification of the functionals in the variational formulation. The Lamé constants $\lambda = \frac{E}{2(1+\nu)}$ and $\mu = \frac{E\nu}{(1+\nu)(1-2\nu)}$ are computed using the values $E = 10$ and $\nu = 0.3$ [37]. The remaining model parameters are given by: $d_1 = 0.05, d_2 = 0.1, D_0 = 1.0, D_1 = 0.1,$ and $\theta_0 = D_0, \theta_2 = \sqrt{2}(D_0 + D_1)$. According to (3.20), the stabilization parameters are taken as $\kappa_1 = \theta_0^2/\theta_2^2, \kappa_2 = \theta_0/\theta_2^2, \kappa_3 = \theta_0/2$ and $\kappa_4 = \theta_0/4$. The convergence of the approximate solutions is assessed by computing errors in the respective norms and experimental rates, that we define as usual

$$
\begin{align*}
e(\sigma) &= \| \sigma - \sigma_h \|_{\text{div},\Omega}, \quad e(\mathbf{u}) = \| \mathbf{u} - \mathbf{u}_h \|_{0,\Omega}, \quad e(\rho) = \| \rho - \rho_h \|_{0,\Omega}, \quad e(t) = \| t - t_h \|_{0,\Omega},
\end{align*}
$$

and

$$
\begin{align*}
e(\sigma) &= \| \sigma - \sigma_h \|_{\text{div},\hat{\Omega}}, \quad e(\mathbf{u}) = \| \mathbf{u} - \mathbf{u}_h \|_{1,\hat{\Omega}}, 
\end{align*}
$$

where $e, \tilde{e}$ denote errors computed on two consecutive meshes of sizes $h, \hat{h}$, respectively. We choose the finite element spaces (5.11) and (5.12), that is $\text{BDM}_{k+1} - P_k - P_k - RT_k - P_k - P_{k+1}$ approximations with $k = 0$ and $k = 1$. Errors and decay rates are summarized in Table 6.1, where we observe that optimal convergence $O(h^{k+1})$ is attained for all fields in their relevant norms. These findings are in agreement with the bounds given by Theorem 5.4. In all cases, Picard steps were required to reach the desired tolerance. Sample solutions are displayed in Fig. 6.1.

Example 2. Next we concentrate on the simulation of microscopic lithiation of an anode. Details on model derivation and physical considerations can be found, for instance, in [9,12,13], whereas the specific settings that motivate this example are summarized in [38]. The domain consists of a truncated sphere of radius 10 $\mu$m, representing the silicon core of a secondary particle (see Fig. 6.3(a)), which we discretize using an unstructured mesh of 104913 tetrahedral elements. For this test we consider lowest order Raviart–Thomas elements for the flux and the concentration gradient, and piecewise polynomials for the concentration (see the method developed in [39]). We assume that the face of the truncated sphere which is closest to the plane $x_1 = 0$ (denoted $\Gamma_{N}$) is in contact with a region of electrolyte, that is, the zone between the sphere and the surrounding cube. On $\Gamma_{N}$ we set zero-flux of lithium and also consider that the anode has an external layer that does not permit displacement of the body, so there we set $\mathbf{u} = \mathbf{0}$. On the remainder of the boundary, $\Gamma_{N} = \Gamma\setminus\Gamma_{N}$, we prescribe a maximum lithium concentration $\phi = \phi_{\text{max}}$ with $\phi_{\text{max}} = 26390$ mol m$^{-3}$, as well as $\sigma_{\nu} = \beta \phi \mathbf{v}$, where $\beta$ is a parameter to be specified later on. We assume that the source term is zero, and the diffusivity is specified as $\theta(\sigma) = D_0 I + D_1 \sigma$ with $D_0 = 1.2 \times 10^{-21}$ m$^2$s$^{-1}$, $D_1 = 3.9e^{-14}$ m$^2$s$^{-1}$, and the elastic material properties of silicon are $E = 60$ GPa and $\nu = 0.25$. Following the referenced models, here the total stress contains a contribution due to lithium concentration. More specifically, we consider $\sigma_{\text{tot}} = \sigma - \beta \phi \mathbf{I}$, with $\beta = \frac{\Omega}{2}(3\lambda + 2\mu)/3$, where $\Omega = 4.926e-6$ m$^3$ mol$^{-1}$ is the partial molar volume. The balance of momentum is then $-\nabla \sigma = -\beta \nabla \phi$, or equivalently $-\nabla \sigma_{\text{tot}} = 0$ and the zero traction boundary condition can be recast as $\sigma_{\text{tot}} \mathbf{n} = \mathbf{0}$ on $\Gamma_{N}$.
invariant to moderate values of $\beta$ and the height of the cylinder is $25 \mu m$. We also observe an increase of the Picard iteration count (where we stress that all fields are normalized). We also observe an increase of the Picard iteration count (where we stress that all fields are normalized).

**Example 1:** Convergence history and Picard iteration count for the augmented $\text{BDM}_{k+1} - P_h - P_k - \text{RT}_k - P_h - P_{k+1}$ approximations with $k = 0, 1$. Here $N$ stands for the number of degrees of freedom associated to the each triangulation $\mathcal{T}_h$.

| $N$ | $h$   | $\varepsilon(\sigma)$ | $r(\sigma)$ | $e(\sigma)$ | $r(\rho)$ | $e(\rho)$ | $r(\rho)$ |
|-----|-------|------------------------|-------------|-------------|-----------|-----------|-----------|
| 129 | 0.7071| 1.36946                | -           | 1.902e-02   | -         | 6.669e-02 | -         |
| 465 | 0.3536| 0.71736                | -           | 9.897e-03   | 0.9422    | 3.412e-02 | 0.9668    |
| 1761| 0.1768| 0.36290                | -           | 4.986e-03   | 0.9884    | 1.716e-02 | 0.9918    |
| 6849| 0.0883| 0.18198                | 0.9957      | 2.499e-03   | 0.9796    | 8.590e-03 | 0.9982    |
| 27009| 0.0441| 0.09106                | 0.9989      | 1.250e-03   | 0.9994    | 4.296e-03 | 0.9996    |
| 107265| 0.0221| 0.04553                | 0.9997      | 6.249e-04   | 0.9999    | 2.148e-03 | 0.9999    |

**Augmented $\text{BDM}_1 - P_0 - P_0 - \text{RT}_0 - P_0 - P_1$ scheme**

| $N$ | $h$   | $\varepsilon(\sigma)$ | $r(\sigma)$ | $e(\sigma)$ | $r(\rho)$ | $e(\rho)$ | $r(\rho)$ |
|-----|-------|------------------------|-------------|-------------|-----------|-----------|-----------|
| 337 | 0.7071| 0.40310                | -           | 5.614e-03   | -         | 1.770e-02 | -         |
| 1265| 0.3536| 0.10681                | 1.9160      | 1.468e-03   | 1.9350    | 4.764e-03 | 1.8940    |
| 4897| 0.1768| 0.02705                | 1.9810      | 3.717e-04   | 1.9820    | 1.224e-03 | 1.9600    |
| 19265| 0.0883| 0.00678                | 1.9960      | 9.324e-05   | 1.9950    | 3.091e-04 | 1.9860    |
| 76417| 0.0441| 0.00169                | 2.0000      | 2.332e-05   | 1.9990    | 7.752e-05 | 1.9950    |
| 304385| 0.0221| 0.00044                | 2.0000      | 5.833e-06   | 2.0000    | 1.940e-05 | 1.9980    |

**Augmented $\text{BDM}_1 - P_1 - P_1 - \text{RT}_1 - P_1 - P_2$ scheme**

| $N$ | $h$   | $\varepsilon(\sigma)$ | $r(\sigma)$ | $e(\sigma)$ | $r(\rho)$ | $e(\rho)$ | $r(\rho)$ |
|-----|-------|------------------------|-------------|-------------|-----------|-----------|-----------|
| 1.345e-02 | - | 4.492e-02 | - | 1.514e-02 | - |
| 3.993e-03 | 1.7520 | 1.284e-02 | 1.8070 | 4.342e-03 | 1.8020 |
| 1.054e-03 | 1.9220 | 3.321e-03 | 1.9510 | 1.56e-03 | 1.9100 |
| 2.684e-04 | 1.9730 | 8.378e-04 | 1.9870 | 2.987e-04 | 1.9520 |
| 6.763e-05 | 1.9890 | 2.100e-04 | 1.9960 | 7.599e-05 | 1.9750 |
| 1.696e-05 | 1.9950 | 5.254e-05 | 1.9990 | 1.917e-05 | 1.9870 |

In order to have a model with fewer chemical and physical parameters, and also to accommodate a model with adimensional units, we proceed to rescale the strong form of the governing equations and testing different deformation regimes to match the expected values found in the literature. We introduce the following parameters: the intrinsic size of the domain $L = 1.6e-5 \text{m}^2$, $\nabla' = \nabla/L$, $\div' = \div/L$, $\phi^* = \phi/\phi_{\text{max}}$, $\mathbf{u}' = \mathbf{u}/L$ and $\sigma' = L^2\sigma$. Thus, taking $D_0 = 1.0e-2D_1L^2$, we reduce the parameters $D_0, D_1, \beta, \Omega$ given above to only $\beta^* = \beta\phi_{\text{max}}/L^2$ and $\alpha = 1.0e-2D_1L^2\phi_{\text{max}}$. Making abuse of notation, we rename $\beta^*$ by $\beta$, $\mathbf{u}'$ by $\mathbf{u}$, and so on. The proper scaling of the parameters implies that the baseline case corresponds to $\beta = 5.0e1$ and $\alpha = 1.0e-3$.

**Fig. 6.3(i)** illustrates the sharp transition between high and low concentrations as lithium diffuses from $I_N$ into the secondary particle. In addition, **Fig. 6.3(c)** shows more pronounced displacements near $I_N$ (which is precisely the region where the silicon is fully lithiated), and the particle swelling is indeed influenced by the lithium gradient distribution. The stress-assisted diffusion mechanism together with the dilatation-dependent source term, also contributes to maintain maximum lithium concentration near $I_N$. This two-way coupling effect implies in turn that the lithium concentration is less important in regions where the secondary particle is clamped.

In **Fig. 6.2** we show different constitutive relations defining $\sigma$ as a function of the first component of the Cauchy stress tensor. The first and third specifications correspond to the functions used in this test and in the accuracy example, respectively, whereas the second relationship has been used in [19] in the context of biological materials. Depending on the values attained by the stress, one could then easily derive the values of the augmentation constants. On the other hand, in **Figs. 6.2(b) and 6.2(c)** we report a study on the influence of different values of the coupling constants $\beta$ and $\alpha$ into the norms of selected solution fields for the elasticity and diffusion problems. We remark that the $L^\infty$-norm of $\mathbf{u}_p$ is practically invariant to moderate values of $\beta$, but it increases abruptly when this parameter approaches 70. Furthermore, the $L^2$-norm of the stress increases linearly with $\beta$. As this constant drives the intensity of the deformation as well as the coupling strength, we also observe an increase in the Picard iteration count (where we stress that all fields are normalized). We also observe an increase of the $L^2$-norm of the concentration gradient with respect to $\alpha$, while for smaller values of $\alpha$ the method produces higher values of the $L^2$-norm of $\hat{\mathbf{u}}$.

**Example 3.** In our last example we test a similar model defined on a perforated cylindrical particle (see a sketch in **Fig. 6.4(a)**). The problem setup has been adapted from [13]. The outer and inner radii of the bases are $5 \mu m$ and $1 \mu m$, respectively, and the height of the cylinder is $25 \mu m$. We discretize the domain using an unstructured mesh of 101907 tetrahedral
Fig. 6.1. Example 1: Lowest-order approximation of stress magnitude $|\sigma_h|$ (a), displacement magnitude $|\mathbf{u}_h|$ (b), relevant component of the rotation $\rho_h$ (c), gradient of concentration $|\mathbf{t}_h|$ (d), diffusive flux $|\mathbf{\tilde{\sigma}}_h|$ (e), and solute concentration $\phi_h$ (f). All fields are plotted on the deformed domain.

Fig. 6.2. Example 2. Approximation of different functions $\vartheta(\sigma)$ varying the $\sigma_{11}$ component (a), normalized $L^2$-norm for $\sigma_h$ and $t_h$, $\ell^\infty$-norm for $\mathbf{u}_h$ and number of Picard iterations needed for different values of $\beta$ with $E = 100$ (b), and normalized $L^2$-norm for $\sigma_h$, $t_h$ and $\mathbf{\tilde{\sigma}}_h$ for five different values of $\alpha$ (c).

elements, and employ the method that uses the lowest-order spaces defined in (5.10), (5.12). In this test we consider that the particle is clamped on the inner wall $I^1$, while zero lithium fluxes are prescribed on $I^B \cup I^1$. Also, we fix a maximum lithium concentration on $I^O$, whereas zero traction will be imposed on $I^B \cup I^O$. We let $E = 10$ GPa, $\nu = 0.3$ and $\Omega = 3.497 \times 10^{-6} \text{ m}^3 \text{ mol}^{-1}$. The diffusive source is zero and the diffusivity tensor and body load source are given by $\vartheta(\sigma) = \alpha I + \alpha^2 \sigma + \alpha^3 \mathbf{\hat{a}}^2$ and $f(\phi) = \beta \mathbf{r} \phi$, respectively, where $\mathbf{r}$ is the radial vector $\mathbf{r} = (x, y, 0)^T$ and $\alpha$, $\beta$ are the adimensional parameters given in Example 2, assuming the values $\alpha = 5.0 \times 10^{-3}$ and $\beta = 75$.

Fig. 6.4 shows the approximate solutions, indicating that the cylindrical particle deforms on the faces and outer radius and having a more important displacement on the faces. Finally, as in Example 2, we observe that the lithium concentration induces the swelling of the cylindrical particle, however as on the faces $I^O$ we now have zero-traction and zero concentration flux conditions coexisting, the lithium concentration is no longer maximal on the outer radius.
Fig. 6.3. Example 2. Schematic representation of domain boundaries on a secondary particle silicone anode (a), lowest-order approximation of stress magnitude $|\sigma_{h}|$ (b), displacement magnitude $|u_{h}|$ (c), rotation components (d, e, f), concentration gradient $|t_{h}|$ (g), diffusive flux $|\sigma_{h}|$ (h), and solute concentration $\phi_{h}$ (i).

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Fig. 6.4. Example 3: Geometry for a perforated cylindrical particle (a), approximate displacement magnitude (b), magnitude of the rows of the approximate Cauchy stress (c, d, e), concentration gradient (f), diffusive flux (g), and concentration (h) shown on a clipped geometry.

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