ERROR ESTIMATES FOR SEMI-DISCRETE FINITE ELEMENT APPROXIMATIONS FOR A MOVING BOUNDARY PROBLEM CAPTURING THE PENETRATION OF DIFFUSANTS INTO RUBBER

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Abstract. We consider a moving boundary problem with kinetic condition that describes the diffusion of solvent into rubber and study semi-discrete finite element approximations of the corresponding weak solutions. We report on both *a priori* and *a posteriori* error estimates for the mass concentration of the diffusants, and respectively, for the *a priori unknown* position of the moving boundary. Our working techniques include integral and energy-based estimates for a nonlinear parabolic problem posed in a transformed fixed domain combined with a suitable use of the interpolation-trace inequality to handle the interface terms. Numerical illustrations of our FEM approximations are within the experimental range and show good agreement with our theoretical investigation. This work is a preliminary investigation necessary before extending the current moving boundary modeling to account explicitly for the mechanics of hyperelastic rods to capture a directional swelling of the underlying elastomer.

Key words. Moving boundary problem, finite element method, method of lines, *a priori* error estimate, *a posteriori* error estimate, diffusion of chemicals into rubber.

1. Introduction

Sharp interfaces moving in an *a priori* unknown way inside materials play a key role in a number of study cases in science and technology, including in the forecast of the durability of cementitious-based materials (cf. e.g. [24, 5, 11, 26]), large-time behavior of chemical species from the environment slowly penetrating by diffusion and swelling rubber-based materials (cf. e.g. [25, 27, 1]), to controlling phase transitions like melting and freezing or solid-solid changes in concrete (cf. e.g. [10, 29, 21]), to mention but a few. Due to the inherent non-linearity of such moving boundary problems, analytical representations of solutions are often either unavailable or not computable. Hence, one has to rely on direct computational approaches to get insight for instance in the behavior of large times of such moving sharp interfaces, as this usually defines the lifetime of the material under investigation.

In the framework of this paper, we study a semi-discrete finite element approximation of weak solutions to a one dimensional moving boundary problem that models the diffusion of solvent into rubber (see Section 2). This is a follow-up study of our recent work [1], where we proposed a finite element approximation of solutions to a moving boundary problem which we used to recover experimental data. Now, we explore the quality of our approximation scheme. Specifically, we report on both *a priori* and *a posteriori* error estimates for the mass concentration of the diffusants, and respectively, for the position of the moving boundary. Our working techniques include integral and energy-based estimates for the corresponding nonlinear parabolic problem posed in a transformed fixed domain, combined with a suitable use of the interpolation-trace inequality to handle the interface terms. At

the technical level, we were very much inspired by the references: [6, 32, 30, 28], and [5]. It is worth noting that similar work has been done in related contexts. For instance, in [24], the authors show the convergence of a numerical scheme obtained by combining an Euler discretization in time with a Scharfetter-Gummel discretization in space for a concrete carbonation model with moving boundary reformulated for a fixed space domain. In [26], A. Zurek studies the long time regime of the moving interface driving the concrete carbonation reaction model by tailoring an implicit in time and finite volume in space scheme. He proves that the approximate free boundary increases in time with $\sqrt{t}$-law as theoretically predicted in [31]. In [23], one develops an adaptive moving mesh method for the numerical solution of an enthalpy formulation of a class of heat-conduction problems with phase change. The main aim of [22] is to provide a comparison of several numerical methods including displacing level sets, moving grids, and diffusing phase fields to address two well-known Stefan problems arising as best formulations for phase transformations like melting of a pure phase and diffusional solid-state phase changes in binary systems.

To handle our problem, we decided to use the finite element method as this fits best to the regularity of the (weak) solutions to our moving boundary problem. Mind though that other discretization methods are likely to be applicable as well. As our work is purely in 1D and no expensive computations are expected, and as, on top of this, we wish to rely on open source facilities, we chose Python for the implementation work.

We present here a preliminary investigation of this class of problems. This is necessary before extending the current moving boundary modeling to account explicitly for the mechanics of hyperelastic rods to capture a directional swelling of the underlying elastomer. In this spirit, a natural next step would be to perform the numerical analysis of a two-scale finite element approximation of the setup described in [25].

The outline of this study is as follows: We formulate our moving boundary problem in Section 2. The discussion of the setting of the model equations is based on [1]. We collect in Section 3 our basic assumptions on parameters and model components, as well as notations and existing preliminary results. Section 4 contains the fixed domain transformation of our problem and the definition of our concept of weak solutions which is then the subject of error approximation estimates investigated here. Benefiting of the mathematical analysis done for our problem in [3, 4], we are able to prove the global existence of weak solutions to the semi-discrete problem and obtain the needed uniform boundedness results to produce convergent numerical schemes. As main result, we obtain *a priori* and *a posteriori* error estimates as listed in Section 5. A couple of numerical experiments are discussed in Section 6. Essentially, they support numerically the available experimental results. Finally, a brief conclusion of this work is outlined in Section 7.

2. Model equations

We consider a thin slab of a dense rubber, denoted by Ω of vertical length $L > 0$, placed in contact with a diffusant reservoir. When the diffusant concentration at the bottom face of the rubber exceeds some threshold, the diffusant moves into the rubber creating a sharp interface that separates the rubber Ω into two parts, the diffusant free region and diffusant-penetrated region. Our region of interest is the diffusant-penetrated part where the diffusant's flux is assumed to satisfy Fick's

law. The actual problem is to find the diffusant concentration profile inside the diffusant-penetrated region and the location of the moving interface separating the penetrated from the not-yet penetrated region. Such a setting is referred to as a one-phase moving boundary problem. Formulations as a two-phase boundary problem are possible as well, but are currently not in our focus; see e.g. [16] for a nicely written textbook regarding modeling with moving interfaces.

In this work, the modeling domain is the onedimensional slab shown in Figure 1, which is the longitudinal line where $0 < s(0) \leq s(t) \leq L$. For a fixed observa-

Diffusant-free rubber at $t = 0$

Zone inside rubber with penetration of diffusants at $t = 0$
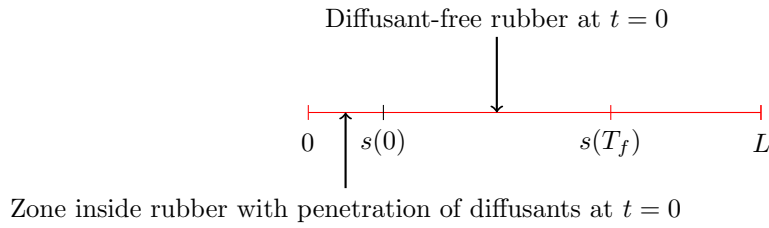
FIGURE 1. Sketch of one dimensional geometry – a macroscopic thin slab made of rubber.

tion time $T_f \in (0, \infty)$, the interval $[0, T_f]$ is the time span of the process we are considering. Let $x \in [0, s(t)]$ and $t \in [0, T_f]$ denote the space and respectively time variable, and let $m(t, x)$ be the concentration of diffusant placed in position x at time t. The diffusants concentration $m(t, x)$ acts in the region $Q_s(T_f)$ defined by

$$Q_s(T_f) := \{(t, x) | t \in (0, T_f) \text{ and } x \in (0, s(t))\}.$$

The problem reads: Find $m(t, x)$ and the position of the moving interface $x = s(t)$ for $t \in (0, T_f)$ such that the couple $(m(t, x), s(t))$ satisfies the following

(1) $$\frac{\partial m}{\partial t} - D\frac{\partial^2 m}{\partial x^2} = 0 \quad \text{in} \quad Q_s(T_f),$$

(2) $$-D\frac{\partial m}{\partial x}(t, 0) = \beta(b(t) - \mathrm{H}m(t, 0)) \quad \text{for} \quad t \in (0, T_f),$$

(3) $$-D\frac{\partial m}{\partial x}(t, s(t)) = s'(t)m(t, s(t)) \quad \text{for} \quad t \in (0, T_f),$$

(4) $$s'(t) = a_0(m(t, s(t)) - \sigma(s(t)) \quad \text{for} \quad t \in (0, T_f),$$

(5) $$m(0, x) = m_0(x) \quad \text{for} \quad x \in [0, s(0)],$$

(6) $$s(0) = s_0 > 0 \text{ with } 0 < s_0 < s(t) < L,$$

where $a_0 > 0$ is a kinetic coefficient, β is a positive constant, $D > 0$ is a diffusion constant, $\mathrm{H} > 0$ is the Henry's constant, σ is a function on $\mathbb{R}$, b is a given boundary function on $[0, T]$, and $s_0 > 0$ is the initial position of the free boundary and m_0 is the initial concentration of the diffusant.

The boundary condition (3) describes the mass conservation of diffusant concentration at the moving boundary. It indicates that the diffusion mechanism is responsible for pushing the interface. In particular (4) points out that the mechanical behaviour (here it is about the swelling of the rubber) also contributes to the motion of the moving penetration front. The explanation of the model equations and the physical meaning of the parameters are given in [1].

3. Notations, assumptions and preliminaries

In this section, we list our basic assumptions on the data, notations as well as approximation properties of functions that are required for the error analysis discussed in the next sections.

3.1. Function spaces and elementary inequalities. Let $u, v : \Omega \to \mathbb{R}$ denote two generic functions. Let $W^{r,p}(\Omega)$ be the Sobolev space on domain Ω for $1 \leq p \leq \infty$ and $r \geq 0$. For $r = 0$, we simply write $L^p(\Omega)$ in place of $W^{0,p}(\Omega)$ with the norm $\|\cdot\|_{L^p(\Omega)}$ defined as follows:

$$\|u\|_{L^p(\Omega)} := \begin{cases} \left(\int_{\Omega} |u(x)|^p dx \right)^{\frac{1}{p}} & \text{for } 1 \leq p < \infty, \\ \text{ess sup}\{|u(x)| : x \in \Omega\} & \text{for } p = \infty, \end{cases}$$

For $p = 2$ and $r \geq 1$, we write $H^r(\Omega)$ in place of $W^{r,2}(\Omega)$ with the norm $\|\cdot\|_{H^r(\Omega)}$ defined by

$$\tag{7} \|u\|_{H^r(\Omega)} = \left(\sum_{|\alpha| \leq r} \int_{\Omega} |\partial^\alpha u|^2 dx \right)^{\frac{1}{2}}.$$

In (7) $\partial^\alpha u$ denotes the α'th derivative of u in the weak sense. Furthermore, for $L^2(\Omega)$ and $H^r(\Omega)$ we have the following inner products.

$$(u, v)_{L^2(\Omega)} := \int_{\Omega} u(x)v(x)dx,$$

$$(u, v)_{H^r(\Omega)} := \sum_{|\alpha| \leq r} (\partial^r u, \partial^r v)_{L^2(\Omega)}.$$

Let X be a Banach space with norm $\|\cdot\|_X$ and $v : [0, T] \to X$ be a function. Correspondingly, $L^p(0, T, X)$ is a Bochner space endowed with the norms

$$\|v\|_{L^p(0,T,X)} := \begin{cases} \left(\int_0^T \|v(\tau)\|_X^p d\tau \right)^{\frac{1}{p}} & \text{for } 1 \leq p < \infty, \\ \sup_{0 \leq \tau \leq T} \|v(\tau)\|_X & \text{for } p = \infty. \end{cases}$$

More information on Sobolev and Bochner spaces with their various norms and inner products can be found for instance in [8, 9]. For the convenience of writing, we denote $u(t, 0)$ and $u(t, 1)$ by $u(0)$ and $u(1)$, respectively. We also use the prime $(')$ to point out the derivative with respect to time variable, and $\|\cdot\|$ and $(\cdot, \cdot)$ for the norm and, respectively, inner product in $L^2(\Omega)$. Furthermore, $\|\cdot\|_\infty$ refers to the norm of $L^\infty(\Omega)$.

We list a few elementary inequalities that we frequently use in this work.

  (i) Young's inequality:

$$\tag{8} ab \leq \xi a^p + c_\xi b^q,$$

     where $a, b \in \mathbb{R}_+$, $\xi > 0$, $c_\xi := \dfrac{1}{q} \dfrac{1}{\sqrt[q]{(\xi p)^q}} > 0$, $\dfrac{1}{p} + \dfrac{1}{q} = 1$ and $p \in (1, \infty)$.

  (ii) Interpolation inequality: For all $u \in H^1(0, 1)$, there exists a constant $\hat{c} > 0$ depending on $\theta \in [\frac{1}{2}, 1)$ such that

$$\tag{9} \|u\|_\infty \leq \hat{c} \|u\|^\theta \|u\|_{H^1(0,1)}^{1-\theta}.$$

For $\theta = 1/2$, one gets

$$\|u\|_\infty^2 \leq \hat{c}\left(\xi\left\|\frac{\partial u}{\partial y}\right\|^2 + (\xi + c_\xi)\|u\|^2\right),$$

where ξ and c_ξ are as in (8). See details in [19] p. 285 (example 21.62).

3.2. Assumptions on parameters. Throughout this paper, we assume the following restrictions on the parameters.

(A1) a_0, H, D, s_0, T_f are positive constants.

(A2) $b \in W^{1,2}(0, T_f)$ with $0 < b_* \leq b \leq b^*$ on $(0, T_f)$, where b_* and b^* are positive constants.

(A3) $\beta \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ such that $\beta = 0$ on $(\infty, 0]$, and there exists $r_\beta > 0$ such that $\beta' > 0$ on $(0, r_\beta)$ and $\beta = k_0$ on $[r_\beta, +\infty)$, where $k_0 > 0$.

(A4) $\sigma \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ such that $\sigma = 0$ on $(-\infty, 0)$, and there exists r_σ such that $\sigma' > 0$ on $(0, r_\sigma)$ and $\sigma = c_0$ on $[r_\sigma, +\infty)$, where c_0 satisfies

$$(10) \qquad\qquad 0 < c_0 < \min\{2\sigma(0), b^*\mathrm{H}^{-1}\}.$$

(A5) $0 < s_0 < r_\sigma$ and $m_0 \in H^1(0, s_0)$ such that $\sigma(0) \leq u_0 \leq b^*\mathrm{H}^{-1}$ on $[0, s_0]$.

The assumptions (A1)–(A5) are adopted from [4], where the authors have proved the global solvability of the problem and continuous dependence estimates of the solution with respect to the initial data.

3.3. Basic facts from approximation theory. Let $N \in \mathbb{N}$ be given. We set $0 = y_0 < y_1 < \cdots < y_{N-1} = 1$ as discretization points in the interval $[0, 1]$. We set $k_i := y_{i+1} - y_i$ for $i \in \{0, 1, \cdots, N-2\}$ and $k := \max\{k_i : i \in \{0, 1, \cdots, N-2\}\}$. We introduce the space

$$(11) \qquad\qquad V_k := \{\nu \in C[0, 1] : \nu|_{[y_j, y_{j+1}]} \in \mathbb{P}_1\},$$

where $\mathbb{P}_1$ represents the set of polynomials of degree one. Let $\{\phi_i\}_{i=0}^{N-1}$ be the set of basis functions for the space V_k defined by

$$\phi_i(y) = \begin{cases} 0 & \text{if} \quad y < y_{i-1} \\ \dfrac{y - y_{i-1}}{k_{i-1}} & \text{if} \quad y_{i-1} \leq y < y_i \\ \dfrac{y_{i+1} - y}{k_i} & \text{if} \quad y_i \leq y < y_{i+1} \\ 0 & \text{if} \quad y_{i+1} \leq y. \end{cases}$$

We define the interpolation operator $I_k : C[0, 1] \to V_k$ by

$$(I_k u)(y) := \sum_{i=0}^{N-1} u(y_i, t)\phi_i(y).$$

Here the function $I_k u$ is called the Lagrange interpolant of u of degree 1; for more details see e.g. [2].

Lemma 3.1. *Take $\theta \in [\frac{1}{2}, 1)$ and $\psi \in H^2(0, 1)$. Then there exist strictly positive constants γ_1, γ_2 and γ_3 such that the Lagrange interpolant $I_k\psi$ of ψ satisfies the following estimates:*

(i) $\|\psi - I_k\psi\| \leq \gamma_1 k^2 \|\psi\|_{H^2(0,1)}$

(ii) $\left\|\dfrac{\partial}{\partial y}(\psi - I_k\psi)\right\| \leq \gamma_2 k \|\psi\|_{H^2(0,1)}$

(iii) $|\psi(0) - I_k\psi(0)| \leq \hat{c}\left(\gamma_1 k^2 + \gamma_3 k^{1+\theta}\right)\|\psi\|_{H^2(0,1)}$

(iv) $|\psi(1) - I_k\psi(1)| \leq \hat{c}\left(\gamma_1 k^2 + \gamma_3 k^{1+\theta}\right)\|\psi\|_{H^2(0,1)}$

Proof. The inequalities (i) and (ii) are standard results. For details on their proof, see for instance page 61 in [2] and page 3 in [17]. To show (iii), we use the interpolation inequality (9) together with (i) and (ii) to obtain

$$|\psi(0) - I_k\psi(0)| \leq \hat{c}\|\psi - I_k\psi\|_{L^2(0,1)}^{\theta}\|\psi - I_k\psi\|_{H^1(0,1)}^{1-\theta}$$

$$\leq \hat{c}\|\psi - I_k\psi\|_{L^2(0,1)}^{\theta}\left(\|\psi - I_k\psi\|^{1-\theta} + \left\|\frac{\partial}{\partial y}(\psi - I_k\psi)\right\|^{1-\theta}\right)$$

$$\leq \hat{c}\left(\gamma_1 k^2 + \gamma_1^\theta\gamma_2^{1-\theta}k^{1+\theta}\right)\|\psi\|_{H^2(0,1)}.$$

Taking $\gamma_3 := \gamma_1^\theta\gamma_2^{1-\theta}$ gives the estimate (iii). A similar argument applied to $\psi(1)$ gives (iv). □

4. Fixed-domain transformation and definition of weak solutions

Firstly, we perform the non-dimensionalization of the model equations (1)–(6). We then transform the non-dimensional model equations from the a priori unknown non-cylinderical domain into the cylinderical domain $Q(T) := \{(\tau, y)|\ \tau \in (0, T)$ and $y \in (0, 1)\}$ by using the Landau transformation $y = x/s(t)$, see for instance [18]. For more details on non-dimensionalization and transformation, we refer the reader to [1] where the preliminary steps are done. In dimensionless form, the transformed problem reads as follows:

$$(12)\qquad \frac{\partial u}{\partial \tau} - y\frac{h'(\tau)}{h(\tau)}\frac{\partial u}{\partial y} - \frac{1}{(h(\tau))^2}\frac{\partial^2 u}{\partial y^2} = 0 \quad \text{in} \quad Q(T),$$

$$(13)\qquad -\frac{1}{h(\tau)}\frac{\partial u}{\partial y}(\tau, 0) = \text{Bi}\left(\frac{b(\tau)}{m_0} - \text{H}u(\tau, 0)\right) \quad \text{for} \quad \tau \in (0, T),$$

$$(14)\qquad -\frac{1}{h(\tau)}\frac{\partial u}{\partial y}(\tau, 1) = h'(\tau)u(\tau, 1) \quad \text{for} \quad \tau \in (0, T),$$

$$(15)\qquad h'(\tau) = A_0\left(u(\tau, 1) - \frac{\sigma(h(\tau))}{m_0}\right) \quad \text{for} \quad \tau \in (0, T)$$

$$(16)\qquad u(0, y) = u_0(y) \quad \text{for} \quad y \in [0, 1],$$

$$(17)\qquad h(0) = h_0.$$

We refer to the system (12)–(17) posed in the cylinderical domain $Q(T)$ as problem (P).

Remark 4.1. *We refer the reader to* [1] *for the definition of dimensionless quantities* u, h, τ, y, T, Bi, A_0. *Here we only mention that* Bi *is the mass transfer Biot number and* A_0 *is the Thiele modulus.*

Definition 4.1. (Weak Solution to (P)). *We call the couple* (u, h) *a weak solution to problem* (P) *on* $S_T := (0, T)$ *if and only if*

$$h \in W^{1,\infty}(S_T) \quad \text{with} \quad h_0 < h(T) \leq L,$$

$$u \in W^{1,2}(Q(T)) \cap L^\infty(S_T, H^1(0, 1)) \cap L^2(S_T, H^2(0, 1)),$$

such that for all $\tau \in S_T$ *the following relations hold*

$$\left(\frac{\partial u}{\partial \tau}, \varphi\right) - \frac{h'(\tau)}{h(\tau)}\left(y\frac{\partial u}{\partial y}, \varphi\right)$$

$$+ \frac{1}{(h(\tau))^2}\left(\frac{\partial u}{\partial y}, \frac{\partial \varphi}{\partial y}\right) - \frac{1}{h(\tau)}\text{Bi}\left(\frac{b(\tau)}{m_0} - \text{H}u(\tau, 0)\right)\varphi(0)$$

$$(18) \qquad + \frac{h'(\tau)}{h(\tau)} u(\tau,1)\varphi(1) = 0 \ \ \textit{for all } \varphi \in H^1(0,1),$$

$$(19) \qquad h'(\tau) = A_0 \left(u(\tau,1) - \frac{\sigma(h(\tau))}{m_0} \right),$$

$$(20) \qquad u(0,y) = u_0(y) \ \ \textit{for } \ y \in [0,1],$$

$$(21) \qquad h(0) = h_0.$$

Theorem 4.1. *If* (A1)–(A5) *hold, then problem* (P) *has a unique solution* (u,h) *on* S_T *in the sense of Definition 4.1.*

Proof. We refer the reader to Theorem 2.4 in [3] for a statement of the local existence of weak solutions to problem (P) and to Theorem 3.3 and Theorem 3.4 in [4] for a way to ensure the global existence and continuous dependence with respect to initial data. $\qquad\square$

We now define the finite element Galerkin approximation to (18)–(21) on the finite dimensional subspace V_k. The semi-discrete approximation u_k and h_k of u and h is now defined to be the mapping $u_k : [0,T] \to V_k$ and $h_k : [0,T] \to \mathbb{R}_+$ such that (22)–(25) holds. We denote the semi-discrete form (22)–(25) of problem (P) by (P_d).

Definition 4.2. (Weak Solution to (P_d)). *We call the couple* (u_k, h_k) *a weak solution to problem* (P_d) *if and only if there is a* $S_T := (0,T)$ *(for some* $T > 0$*) such that*

$$h_k \in W^{1,\infty}(S_T) \ \ \text{with} \ h_0 < h_k(T) \le L$$
$$u_k \in H^1(S_T, V_k) \cap L^2(S_T, H^1(0,1)) \cap L^\infty(S_T, L^2(0,1))$$

and for all $\tau \in S_T$ *it holds*

$$\left(\frac{\partial u_k}{\partial \tau}, \varphi_k \right) - \frac{h_k'(\tau)}{h_k(\tau)} \left(y \frac{\partial u_k}{\partial y}, \varphi_k \right)$$
$$+ \frac{1}{(h_k(\tau))^2} \left(\frac{\partial u_k}{\partial y}, \frac{\partial \varphi_k}{\partial y} \right) - \frac{1}{h_k(\tau)} \text{Bi} \left(\frac{b(\tau)}{m_0} - \text{H} u_k(\tau,0) \right) \varphi_k(0)$$

$$(22) \qquad + \frac{h_k'(\tau)}{h_k(\tau)} u_k(\tau,1)\varphi_k(1) = 0 \ \ \textit{for all } \ \varphi_k \in V_k,$$

$$(23) \qquad h_k'(\tau) = A_0 \left(u_k(\tau,1) - \frac{\sigma(h_k(\tau))}{m_0} \right),$$

$$(24) \qquad u_k(0) = u_{0,k}(y) \ \text{ for } \ y \in [0,1],$$

$$(25) \qquad h_k(0) = h_0.$$

Lemma 4.1. *Assume* (A1)–(A5) *hold. Then there exist a time* $\hat{T} \in (0,T]$ *and positive constants* L, M_1, M_2 *(not depending on* k*) such that for a.e.* $\tau \in (0,\hat{T})$ *the following inequalities hold true for the pair* (u_k, h_k) *arising in Definition 4.2:*

(i) $0 < h_0 \le h_k(\tau) \le L$
(ii) $0 < u_k(\tau, y) < M_1$
(iii) $|h_k'(\tau)| \le M_2$.

Proof. (i) is built in the concept of weak solution detailed in Definition 4.2. It does not require a proof. We added it here simply to stress the importance of the fact the we work exclusively in a bounded moving domain. (ii) is the main statement here. This holds true as a consequence of the fact that the space continuous version

of the statement (i.e. $0 < u(\tau, y) < M_1$) holds true; we rely on the arguments of
the proof of Theorem 3.1 in [4], combined with the fact that the treated geometry
is one dimensional. Hence, $\hat{T} > 0$ is possibly small, which is sufficient for deriving
our next results. Note though that a discrete version of the Stampacchia trick,
worked out with details in [33], can potentially be applied here as well in order to
replace the local time $\hat{T}$ with a maximal time. Alternative arguments employing
the structure of the problem as in [35] or based on linear simplicial finite elements
as in [34] can also be used in principle. (iii) is a direct consequence of (i) and (ii)
combined with (23).

$\square$

Theorem 4.2. *Let the hypothesis of Lemma 4.1 be fulfilled. Then it exists a unique
solution*

$$(u_k, h_k) \in H^1(S_{\hat{T}}, V_k) \cap L^2(S_{\hat{T}}, H^1(0,1)) \cap L^\infty(S_{\hat{T}}, L^2(0,1)) \times W^{1,\infty}(S_{\hat{T}})$$

*in the sense of Definition 4.2. Furthermore, there exists a constant $\tilde{c} > 0$ (indepen-
dent of k) such that*

$$(26) \qquad \max_{0 \leq \tau \leq \hat{T}} \|u_k\|_{L^2(0,1)}^2 + \int_0^{\hat{T}} \left\| \frac{\partial u_k}{\partial y} \right\|_{L^2(0,1)}^2 d\tau \leq \tilde{c}.$$

Proof. Let V_k be the finite dimensional subspace defined in (11) constructed based
on the span of the hat functions $\{\phi_j\}, j \in \{0, 1, \cdots, N-1\}$. Let $\alpha_j : (0, \hat{T}) \to \mathbb{R}$
denote the Galerkin projection coefficient for jth degree of freedom. Then the
finite-dimensional Galerkin approximation of the function u is defined by

$$u_k(\tau, y) := \sum_{j=0}^{N-1} \alpha_j(\tau) \phi_j(y),$$

where the coefficients $\alpha_j(\tau)$, $j \in \{0, 1, \ldots N-1\}$ are determined by the following
relations:

$$\left(\frac{\partial u_k}{\partial \tau}, \varphi_k \right) - \frac{h_k'(\tau)}{h_k(\tau)} \left(y \frac{\partial u_k}{\partial y}, \varphi_k \right) + \frac{1}{(h_k(\tau))^2} \left(\frac{\partial u_k}{\partial y}, \frac{\partial \varphi_k}{\partial y} \right)$$

$$(27) \qquad - \frac{1}{h_k(\tau)} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} - \mathrm{H} u_k(\tau, 0) \right) \varphi_k(0) + \frac{h_k'(\tau)}{h_k(\tau)} u_k(\tau, 1) \varphi_k(1) = 0,$$

$$(28) \qquad h_k'(\tau) = A_0 \left(u_k(\tau, 1) - \frac{\sigma(h_k(\tau))}{m_0} \right), \quad \tau \in (0, \hat{T})$$

for all $\varphi_k \in \mathrm{span}\{\phi_j\}$, $j \in \{0, 1, \cdots, N-1\}$ and

$$(29) \qquad \alpha_j(0) = (u_{0,k}, \phi_j),$$

$$(30) \qquad h_k(0) = h_0.$$

Taking in (27) and (28) as test function $\varphi_k = \phi_j$ for $j \in \{0, 1, \cdots, N-1\}$, we
obtain the following system of ordinary differential equations for the unknown $\alpha = (\alpha_j)_{j=0,1,\cdots,N-1}$ and h_k:

$$\sum_{i=0}^{N-1} M_i \alpha_i'(\tau) - \frac{h_k'}{h_k} \sum_{i=0}^{N-1} K_i \alpha_i + \frac{1}{h_k^2} \sum_{i=0}^{N-1} A_i \alpha_i$$

$$(31) \qquad \qquad = \frac{1}{h_k} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} \phi(0) - \mathrm{H}\alpha \right) - \frac{h_k'}{h_k} \alpha =: G_1(\alpha, h_k),$$

$$(32) \qquad h_k'(\tau) = A_0 \left(\sum_{i=0}^{N-1} \alpha_i \phi_i(1) - \frac{\sigma(h_k(\tau))}{m_0} \right) =: G_2(\alpha, h_k),$$

where

$$(33) \qquad (M_i)_j := \int_0^1 \phi_i \phi_j dy,$$

$$(34) \qquad (K_i)_j := \int_0^1 y \frac{\partial \phi_i}{\partial y} \phi_j dy,$$

$$(35) \qquad (A_i)_j := \int_0^1 \frac{\partial \phi_i}{\partial y} \frac{\partial \phi_j}{\partial y} dy.$$

Firstly, we prove that G_2 is Lipschitz. Let (α, h_k) and $(\beta, \tilde{h}_k)$ be two pairs.

$$\left| G_2(\alpha, h_k) - G_2(\beta, \tilde{h}_k) \right|$$

$$(36) \qquad \leq A_0 \left(\sum_{i=0}^{N-1} |\alpha_i(\tau) - \beta_i(\tau)| \, |\phi_i(1)| + \frac{1}{m_0} \left| \sigma(h_k(\tau)) - \sigma(\tilde{h}_k(\tau)) \right| \right).$$

Using (A4) in (36), we get

$$\left| G_2(\alpha, h_k) - G_2(\beta, \tilde{h}_k) \right| \leq A_0 \left(\sum_{i=0}^{N-1} |\alpha_i(\tau) - \beta_i(\tau)| \, |\phi_i(1)| + \frac{\mathcal{L}}{m_0} \left| h_k(\tau) - \tilde{h}_k(\tau) \right| \right)$$

$$\leq \mathcal{M} \left(\sum_{i=0}^{N-1} |\alpha_i(\tau) - \beta_i(\tau)| + \left| h_k(\tau) - \tilde{h}_k(\tau) \right| \right)$$

$$= \mathcal{M} |(\alpha, h_k) - (\beta, \tilde{h}_k)|,$$

where $\mathcal{L}$ is a Lipschitz constant and

$$\mathcal{M} := \max \left\{ A_0 \max_{0 \leq i \leq N-1} |\phi_i(1)|, \frac{A_0 \mathcal{L}}{m_0} \right\}.$$

Thus, G_2 is Lipschitz. Now, we show that G_1 is Lipschitz.

$$G_1(\alpha, h_k) - G_1(\beta, \tilde{h}_k) = \text{Bi} \frac{b(\tau)}{m_0} \left(\frac{1}{h_k} - \frac{1}{\tilde{h}_k} \right) \phi(0)$$

$$(37) \qquad - \text{Bi} \, \text{H} \left(\frac{\alpha}{h_k} - \frac{\beta}{\tilde{h}_k} \right) - \left(\frac{h_k'}{h_k} \alpha - \frac{\tilde{h}_k'}{\tilde{h}_k} \beta \right).$$

Using (A2) in (37) yields

$$\left| G_1(\alpha, h_k) - G_1(\beta, \tilde{h}_k) \right| \leq \text{Bi} \frac{b^*}{m_0 h_k \tilde{h}_k} |h_k - \tilde{h}_k| |\phi(0)|$$

$$+ \text{Bi} \, \text{H} \left| \frac{\alpha}{h_k} - \frac{\beta}{\tilde{h}_k} \right| + \left| \frac{h_k'}{h_k} \alpha - \frac{\tilde{h}_k'}{\tilde{h}_k} \beta \right|$$

$$= \sum_{\ell=1}^3 I_\ell,$$

where

$$I_1 := \text{Bi} \frac{b^*}{m_0 h_k \tilde{h}_k} |h_k - \tilde{h}_k| |\phi(0)| \leq \text{Bi} \frac{b^*}{m_0 h_k \tilde{h}_k} |h_k - \tilde{h}_k|,$$

$$I_2 := \mathrm{Bi}\,\mathrm{H}\left|\frac{\alpha}{h_k} - \frac{\beta}{\tilde{h}_k}\right| \le \mathrm{Bi}\,\mathrm{H}\left(|\alpha|\frac{|h_k - \tilde{h}_k|}{h_k\tilde{h}_k} + \frac{|\alpha - \beta|}{\tilde{h}_k}\right),$$

$$\begin{aligned}
I_3 &:= \left|\frac{h_k'}{h_k}\alpha - \frac{\tilde{h}_k'}{\tilde{h}_k}\beta\right|\\
&= \left|h_k'\left(\frac{\alpha}{h_k} - \frac{\beta}{\tilde{h}_k}\right) + \frac{\beta}{\tilde{h}_k}\left(h_k' - \tilde{h}_k'\right)\right|\\
&\le |h_k'|\left|\frac{\alpha}{h_k} - \frac{\beta}{\tilde{h}_k}\right| + \mathcal{L}\frac{|\beta|}{|\tilde{h}_k|}\left|h_k - \tilde{h}_k\right|\\
&\le |h_k'|\left(|\alpha|\frac{|h_k - \tilde{h}_k|}{h_k\tilde{h}_k} + \frac{|\alpha - \beta|}{\tilde{h}_k}\right) + \mathcal{L}\frac{|\beta|}{|\tilde{h}_k|}\left|h_k - \tilde{h}_k\right|.
\end{aligned}$$

This shows that G_1 is Lipschitz continuous. By standard arguments for systems of ordinary differential equations, the problem (29)-(32) has a unique solution

$$(\alpha, h_k) \in C^1([0, \hat{T}])^N \times W^{1,\infty}(0, \hat{T}).$$

We now prove the uniform estimate for the solution u to the finite dimensional problem.

Taking $\varphi = u_k$ in (27) yields

$$\begin{aligned}
\frac{1}{2}\frac{d}{d\tau}\|u_k(\tau)\|^2 &+ \frac{1}{(h_k(\tau))^2}\left\|\frac{\partial u_k(\tau)}{\partial y}\right\|^2 = \int_0^1 \frac{h_k'}{h_k}y\frac{\partial u_k}{\partial y}u_k dy\\
(38)\qquad &+ \frac{1}{h_k(\tau)}\mathrm{Bi}\left(\frac{b(\tau)}{m_0} - \mathrm{H}u_k(\tau,0)\right)u_k(\tau,0) + \frac{h_k'(\tau)}{h_k(\tau)}u_k(\tau,1)u_k(\tau,1).
\end{aligned}$$

Using Hölders inequality for the first term on the right hand side of (38), it holds that

$$\begin{aligned}
\frac{1}{2}\frac{d}{d\tau}\|u_k(\tau)\|^2 &+ \frac{1}{(h_k(\tau))^2}\left\|\frac{\partial u_k(\tau)}{\partial y}\right\|^2 \le \frac{|h_k'|}{h_k}\left\|\frac{\partial u_k}{\partial y}\right\|_{L^2(\Omega)}\|u_k\|_{L^2(\Omega)}\\
(39)\qquad &+ \frac{\mathrm{Bi}}{h_k}\frac{b^*}{m_0}|u_k(\tau,0)| + \frac{|h_k'|}{h_k}|u_k(\tau,1)|^2.
\end{aligned}$$

We note here that, by the Sobolev's embedding inequality in one space dimension, it holds

$$(40)\quad |\vartheta(\tau,y)|^2 \le C_e\|\vartheta(\tau)\|_{H^1(0,1)}\|\vartheta(\tau)\|_{L^2(0,1)} \quad \text{for } \vartheta \in H^1(0,1) \text{ and } y \in [0,1],$$

where C_e is a positive constant. Using (40), the third term on the right hand side of (39) becomes

$$\begin{aligned}
\frac{|h_k'|}{h_k}|u_k(\tau,1)|^2 &\le C_e\frac{\|h_k'\|_{L^\infty(S_{\hat{T}})}}{h_0}\|u_k(\tau)\|_{H^1(0,1)}\|u_k(\tau)\|_{L^2(0,1)}\\
(41)\qquad &\le C_e\frac{\|h_k'\|_{L^\infty(S_{\hat{T}})}}{h_0}\left(\left\|\frac{\partial u_k(\tau)}{\partial y}\right\|_{L^2(0,1)}\|u_k(\tau)\|_{L^2(0,1)} + \|u_k(\tau)\|_{L^2(0,1)}^2\right).
\end{aligned}$$

Using (41), (39) becomes

$$\begin{aligned}
\frac{1}{2}\frac{d}{d\tau}\|u_k\|^2 &+ \frac{1}{(h_k)^2}\left\|\frac{\partial u_k}{\partial y}\right\|^2 \le (1 + C_e)\frac{\|h_k'\|_{L^\infty(S_{\hat{T}})}}{h_0}\left\|\frac{\partial u_k}{\partial y}\right\|_{L^2(0,1)}\|u_k\|_{L^2(0,1)}\\
(42)\qquad &+ C_e\frac{\|h_k'\|_{L^\infty(S_{\hat{T}})}}{h_0}\|u_k\|_{L^2(0,1)}^2 + \frac{1}{h_0}\frac{b^*}{m_0}\|u_k\|_{H^1(0,1)}.
\end{aligned}$$

Using Young's inequality, (42) leads to

$$
\frac{1}{2}\frac{d}{d\tau}\|u_k\|^2 + \frac{1}{2L^2}\left\|\frac{\partial u_k}{\partial y}\right\|^2 \leq (1 + C_e)\frac{\|h'_k\|_{L^\infty(S_{\hat{T}})}}{h_0}\left(\xi\left\|\frac{\partial u_k}{\partial y}\right\|^2_{L^2(0,1)} + c_\xi\|u_k\|^2_{L^2(0,1)}\right)
$$
$$
+ C_e\frac{\|h'_k\|_{L^\infty(S_{\hat{T}})}}{h_0}\|u_k\|^2_{L^2(0,1)} + \xi\left\|\frac{\partial u_k}{\partial y}\right\|^2_{L^2(0,1)}
$$
$$
+ \xi\|u_k\|^2_{L^2(0,1)} + \frac{c_\xi}{h_0^2}\frac{(b^*)^2}{m_0^2}.
$$

Finally, we get the following inequality

$$
(43) \qquad \frac{1}{2}\frac{d}{d\tau}\|u_k\|^2 + M_1\left\|\frac{\partial u_k}{\partial y}\right\|^2 \leq M_2\|u_k\|^2_{L^2(0,1)} + M_3,
$$

where

$$
M_1 := \frac{1}{2L^2} - \left((1 + C_e)\frac{\|h'_k\|_{L^\infty(S_{\hat{T}})}}{h_0} + 1\right)\xi,
$$
$$
M_2 := \frac{\|h'_k\|_{L^\infty(S_{\hat{T}})}}{h_0}(c_\xi + C_e(c_\xi + 1)) + \xi,
$$
$$
M_3 := \frac{c_\xi}{h_0^2}\frac{(b^*)^2}{m_0^2}.
$$

Choosing a sufficiently small ξ with $M_1 > 0$ and then applying Gronwall's inequality gives the following inequality holds

$$
(44) \qquad \|u_k(\tau)\|^2 \leq c(\hat{T}, h_0, C_e)\left(\|u_k(0)\|^2 + M_3\hat{T}\right),
$$

for all $0 \leq \tau \leq \hat{T}$. Since $\|u_k(0)\|^2 \leq \|u_{0,k}\|^2$, (44) yields

$$
(45) \qquad \max_{0 \leq \tau \leq \hat{T}}\|u_k(\tau)\|^2 \leq \tilde{c}.
$$

Integrating (43) from 0 to $\hat{T}$ and employ the inequality (45) to get

$$
\int_0^{\hat{T}}\left\|\frac{\partial u_k}{\partial y}\right\|^2 d\tau \leq \tilde{c}.
$$

This concludes the proof of (26). $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Remark 4.2. *The entries of the matrices M, K and A given in (33), (34) and (35) are computed explicitly benefiting of the structure of the basis elements $\phi_j \in V_k$, usually piecewise polynomials of some preset degree defined in Ω; see [1] for the explicit form of the matrix K and A when using as basis piecewise linear functions.*

5. Main results

In this Section, we prove *a priori* and *a posteriori* error estimates between the weak solution to (P) and weak solution to a semi-discrete version of (P). The discretization in space is done via the finite element method [2].

Theorem 5.1. *(A priori error estimate) Assume (A1)–(A5) hold. Additionally, take $u_0 \in H^2(0,1)$. Let (u,h) and (u_k, h_k) be the corresponding weak solutions to problem (P) and (P_d) in the sense of Definition 4.1 and Definition 4.2, respectively. Then there exists a constant $c > 0$ (not depending on k) such that*

$$
(46) \qquad \|u - u_k\|^2_{L^\infty(S_{\hat{T}}, L^2(0,1))) \cap L^2(S_{\hat{T}}, H^1(0,1))} + \|h - h_k\|^2_{H^1(S_{\hat{T}})} \leq ck^2.
$$

Proof. We consider the time interval $S_{\hat{T}}$ on which both continuous and discrete solutions to (12)–(17) exist and are uniquely defined. Let $e := u - u_k$ and $h - h_k$ be the pointwise errors of the approximation. By subtracting (22) from (18) and choosing $\varphi = v_k \in V_k$, we obtain the following identity:

$$\left(\frac{\partial u}{\partial \tau}, v_k\right) - \left(\frac{\partial u_k}{\partial \tau}, v_k\right) + \frac{1}{h^2}\left(\frac{\partial u}{\partial y}, \frac{\partial v_k}{\partial y}\right)$$

$$- \frac{1}{h_k^2}\left(\frac{\partial u_k}{\partial y}, \frac{\partial v_k}{\partial y}\right) - \left(\frac{h'}{h}\int_0^1 y\frac{\partial u}{\partial y}v_k dy - \frac{h'_k}{h_k}\int_0^1 y\frac{\partial u_k}{\partial y}v_k dy\right)$$

$$+ \frac{h'}{h}u(\tau,1)v_k(1) - \frac{h'_k}{h_k}u_k(\tau,1)v_k(1)$$

$$(47) \qquad - \frac{1}{h}\text{Bi}\left(\frac{b(\tau)}{m_0} - \text{H}u(\tau,0)\right)v_k(0) + \frac{1}{h_k}\text{Bi}\left(\frac{b(\tau)}{m_0} - \text{H}u_k(\tau,0)\right)v_k(0) = 0,$$

which holds for all $v_k \in V_k$ and for almost every $\tau \in S_{\hat{T}}$.

Arranging conveniently the terms in (47) yields

$$\left(\frac{\partial e}{\partial \tau}, v_k\right) + \frac{1}{h^2}\left(\frac{\partial e}{\partial y}, \frac{\partial v_k}{\partial y}\right) - \left(\frac{1}{h_k^2} - \frac{1}{h^2}\right)\left(\frac{\partial u_k}{\partial y}, \frac{\partial v_k}{\partial y}\right)$$

$$- \left(\frac{h'}{h}\int_0^1 y\frac{\partial e}{\partial y}v_k dy + \left(\frac{h'}{h} - \frac{h'_k}{h_k}\right)\int_0^1 y\frac{\partial u_k}{\partial y}v_k dy\right)$$

$$+ \frac{h'}{h}e(\tau,1)v_k(1) + \left(\frac{h'}{h} - \frac{h'_k}{h_k}\right)u_k(\tau,1)v_k(1)$$

$$(48) \qquad - \left(\text{Bi}\frac{b(\tau)}{m_0}\left(\frac{1}{h} - \frac{1}{h_k}\right)v_k(0) - \text{Bi H}\left(\frac{u(\tau,0)}{h} - \frac{u_k(\tau,0)}{h_k}\right)v_k(0)\right) = 0.$$

In (48), we take as test function $v_k := w_k - u_k \in V_k$ and use the decomposition $v_k = (w_k - u) + e$. Then (48) becomes

$$\left(\frac{\partial e}{\partial \tau}, e\right) + \left(\frac{\partial e}{\partial \tau}, w_k - u\right) + \frac{1}{h^2}\left(\frac{\partial e}{\partial y}, \frac{\partial e}{\partial y}\right)$$

$$+ \frac{1}{h^2}\left(\frac{\partial e}{\partial y}, \frac{\partial}{\partial y}(w_k - u)\right) - \left(\frac{1}{h_k^2} - \frac{1}{h^2}\right)\left(\frac{\partial u_k}{\partial y}, \frac{\partial}{\partial y}(w_k - u_k)\right)$$

$$- \left(\frac{h'}{h}\int_0^1 y\frac{\partial e}{\partial y}(w_k - u_k)dy + \left(\frac{h'}{h} - \frac{h'_k}{h_k}\right)\int_0^1 y\frac{\partial u_k}{\partial y}(w_k - u_k)dy\right)$$

$$+ \frac{h'}{h}e(\tau,1)(w_k(1) - u_k(1)) + \left(\frac{h'}{h} - \frac{h'_k}{h_k}\right)u_k(\tau,1)(w_k(1) - u_k(1))$$

$$- \text{Bi}\frac{b(\tau)}{m_0}\left(\frac{1}{h} - \frac{1}{h_k}\right)(w_k(0) - u_k(0))$$

$$+ \text{Bi H}\left(\frac{u(\tau,0)}{h} - \frac{u_k(\tau,0)}{h_k}\right)(w_k(0) - u_k(0)) = 0.$$

Therefore, we can write

$$\frac{1}{2}\frac{d}{d\tau}\|e\|^2 + \frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 \leq \left\|\frac{\partial e}{\partial \tau}\right\|\|u - w_k\| + \frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|\left\|\frac{\partial}{\partial y}(u - w_k)\right\|$$

$$+ |h - h_k|\frac{h + h_k}{h^2 h_k^2}\left\|\frac{\partial u_k}{\partial y}\right\|\left\|\frac{\partial}{\partial y}(w_k - u_k)\right\|$$

$$+ \frac{h'}{h}\left\|\frac{\partial e}{\partial y}\right\|\|w_k - u_k\| + \left|\frac{h'}{h} - \frac{h'_k}{h_k}\right|\left\|\frac{\partial u_k}{\partial y}\right\|\left\|\frac{\partial}{\partial y}(w_k - u_k)\right\|$$

$$+ \frac{h'}{h}|e(\tau,1)||(w_k(1) - u(1)) + e(\tau,1)|$$

$$+ \left|\frac{h'}{h} - \frac{h_k'}{h_k}\right| |u_k(\tau,1)||(w_k(1) - u(1)) + e(\tau,1)|$$

$$+ \mathrm{Bi}\frac{b^*}{m_0}\left|\frac{1}{h} - \frac{1}{h_k}\right||w_k(0) - u_k(0)|$$

(49)
$$+ \mathrm{Bi\,H}\left|\frac{u(\tau,0)}{h} - \frac{u_k(\tau,0)}{h_k}\right||w_k(0) - u_k(0)|.$$

To bound some terms on the right hand side in (49), we introduce the strictly positive constant $c_\ell < \infty, \ell \in \{1,2,\cdots,5\}$. The value for these constants is not explicitly written, but can be calculated. Before proceeding further, we collect two useful estimates in Remark 5.1.

Remark 5.1. *There exist constants c_2, $c_5 > 0$ such that*

(1) $\left|\dfrac{h'}{h} - \dfrac{h_k'}{h_k}\right| \le c_2(|h - h_k| + |h' - h_k'|)$

(2) $\left(\dfrac{u(0)}{h} - \dfrac{u_k(0)}{h_k}\right) = \dfrac{1}{h}(e(0)) + \dfrac{u_k(0)}{h_k}(h_k - h) \le c_5(|e(0)| + |h - h_k|).$

Making use of Remark 5.1, (49) becomes

$$\frac{1}{2}\frac{d}{d\tau}\|e\|^2 + \frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 \le \left\|\frac{\partial e}{\partial \tau}\right\|\|u - w_k\| + \frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|\left\|\frac{\partial}{\partial y}(u - w_k)\right\|$$

$$+ c_1|h - h_k|\left\|\frac{\partial u_k}{\partial y}\right\|\left(\left\|\frac{\partial}{\partial y}(w_k - u)\right\| + \left\|\frac{\partial e}{\partial y}\right\|\right)$$

$$+ \frac{h'}{h}\left\|\frac{\partial e}{\partial y}\right\|(\|w_k - u\| + \|e\|)$$

$$+ c_2(|h - h_k| + |h' - h_k'|)\left\|\frac{\partial u_k}{\partial y}\right\|\left(\left\|\frac{\partial}{\partial y}(w_k - u)\right\| + \left\|\frac{\partial e}{\partial y}\right\|\right)$$

$$+ \frac{h'}{h}|e(1)|(|w_k(1) - u(1)| + |e(1)|)$$

$$+ c_3(|h - h_k| + |h' - h_k'|)|u_k(\tau,1)|(|w_k(1) - u(1)| + |e(1)|)$$

$$+ c_4\mathrm{Bi}\frac{b^*}{m_0}|h - h_k|(|w_k(0) - u(0)| + |e(0)|)$$

$$+ c_5\mathrm{Bi\,H}(|e(0)| + |h - h_k|)(|w_k(0) - u(0)| + |e(0)|) = \sum_{\ell=1}^{9} I_\ell.$$

We set $w_k := I_k u$, where $I_k u$ is the Lagrange interpolation of u. By using Lemma 3.1, Young's inequality (8) and interpolation inequality (9), we obtain the following estimates:

$$I_1 := \left\|\frac{\partial e}{\partial \tau}\right\|\|u - w_k\| \le \left\|\frac{\partial e}{\partial \tau}\right\|\gamma_1 k^2\|u\|_{H^2(0,1)} \le \frac{1}{2}\left\|\frac{\partial e}{\partial \tau}\right\|^2 k^2 + \frac{\gamma_1^2 k^2}{2}\|u\|_{H^2(0,1)}^2,$$

$$I_2 := \frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|\left\|\frac{\partial}{\partial y}(u - w_k)\right\| \le \frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|\gamma_2 k\|u\|_{H^2(0,1)}$$

$$\le \frac{\xi}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + c_\xi\gamma_2^2 k^2\frac{1}{h^2}\|u\|_{H^2(0,1)}^2,$$

$$I_3 := c_1|h - h_k| \left\| \frac{\partial u_k}{\partial y} \right\| \left(\left\| \frac{\partial}{\partial y}(w_k - u) \right\| + \left\| \frac{\partial e}{\partial y} \right\| \right)$$

$$\leq c_1|h - h_k| \left\| \frac{\partial u_k}{\partial y} \right\| \left(\gamma_2 k \left\| u \right\|_{H^2(0,1)} + \left\| \frac{\partial e}{\partial y} \right\| \right)$$

$$\leq \rho|h - h_k|^2 \left\| \frac{\partial u_k}{\partial y} \right\|^2 + c_\rho c_1^2 \gamma_2^2 k^2 \left\| u \right\|_{H^2(0,1)}^2$$

$$+ c_{\hat{\rho}} c_1^2 |h - h_k|^2 \left\| \frac{\partial u_k}{\partial y} \right\|^2 h^2 + \hat{\rho} \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2.$$

We observe that if $u_0 \in H^1(0,1)$, then it also holds that $u_k \in H^1(S_{\hat{T}}, V_k)$. Hence, we can control terms like $\left\| \frac{\partial u_k}{\partial y} \right\|^2$ via

$$(50) \qquad \max_{0 \leq \tau \leq \hat{T}} \left\| u_k \right\|_{H^1(0,1)}^2 + \int_0^{\hat{T}} \left\| u_k \right\|_{H^2(0,1)}^2 d\tau \leq \hat{c}_1.$$

Therefore, we get

$$I_3 \leq \rho \hat{c}_1 |h - h_k|^2 + c_\rho c_1^2 \gamma_2^2 k^2 \left\| u \right\|_{H^2(0,1)}^2 + c_{\hat{\rho}} \hat{c}_1 c_1^2 |h - h_k|^2 h^2 + \hat{\rho} \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2,$$

$$I_4 := \frac{h'}{h} \left\| \frac{\partial e}{\partial y} \right\| (\left\| w_k - u \right\| + \left\| e \right\|)$$

$$\leq \frac{h'}{h} \left\| \frac{\partial e}{\partial y} \right\| \left(\gamma_1 k^2 \left\| u \right\|_{H^2(0,1)} + \left\| e \right\| \right)$$

$$\leq \zeta \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 + c_\zeta (h')^2 \left(\gamma_1 k^2 \left\| u \right\|_{H^2(0,1)} + \left\| e \right\| \right)^2$$

$$\leq \zeta \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 + 2c_\zeta (h')^2 \left(\gamma_1^2 k^4 \left\| u \right\|_{H^2(0,1)}^2 + \left\| e \right\|^2 \right),$$

$$I_5 := c_2(|h - h_k| + |h' - h_k'|) \left\| \frac{\partial u_k}{\partial y} \right\| \left(\left\| \frac{\partial}{\partial y}(w_k - u) \right\| + \left\| \frac{\partial e}{\partial y} \right\| \right)$$

$$\leq c_2(|h - h_k| + |h' - h_k'|) \left\| \frac{\partial u_k}{\partial y} \right\| \left(\gamma_2 k \left\| u \right\|_{H^2(0,1)} + \left\| \frac{\partial e}{\partial y} \right\| \right)$$

$$\leq \xi \left(|h - h_k|^2 \left\| \frac{\partial u_k}{\partial y} \right\|^2 + |h' - h_k'|^2 \left\| \frac{\partial u_k}{\partial y} \right\|^2 \right) + c_\xi c_2^2 \gamma_2^2 k^2 \left\| u \right\|_{H^2(0,1)}^2$$

$$+ \hat{\xi} \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 + c_{\hat{\xi}} c_2^2 h^2 \left(|h - h_k|^2 \left\| \frac{\partial u_k}{\partial y} \right\|^2 + |h' - h_k'|^2 \left\| \frac{\partial u_k}{\partial y} \right\|^2 \right),$$

$$\leq \xi \hat{c}_1 \left(|h - h_k|^2 + |h' - h_k'|^2 \right) + c_\xi c_2^2 \gamma_2^2 k^2 \left\| u \right\|_{H^2(0,1)}^2$$

$$+ \hat{\xi} \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 + c_{\hat{\xi}} \hat{c}_1 c_2^2 h^2 \left(|h - h_k|^2 + |h' - h_k'|^2 \right),$$

$$I_6 := \frac{h'}{h} |e(1)|(|w_k(1) - u(1)| + |e(1)|)$$

$$= \frac{h'}{h} |e(1)|^2 + \frac{h'}{h} |e(1)||w_k(1) - u(1)|$$

$$= \frac{h'}{h} |e(1)|^2 + \frac{h'}{h} \left(\frac{|e(1)|^2}{2} + \frac{|w_k(1) - u(1)|^2}{2} \right)$$

$$= \frac{3}{2}\frac{h'}{h}|e(1)|^2 + \frac{h'}{h}\frac{|w_k(1) - u(1)|^2}{2}$$

$$\leq \frac{3}{2}\frac{h'}{h}\hat{c}\,\|e\|^{2\theta}\,\|e\|^{2(1-\theta)}_{H^1(0,1)} + \frac{h'}{2h}\left(\gamma_1 k^2 + \gamma_3 k^{1+\theta}\right)^2 \|u\|^2_{H^2(0,1)}$$

$$\leq \frac{3}{2}\left(\frac{\xi}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + (\frac{\xi}{h^2} + c_\xi \hat{c}^2 (h')^2)\,\|e\|^2\right) + \frac{h'}{2h}\hat{c}^2\left(\gamma_1 k^2 + \gamma_3 k^{1+\theta}\right)^2 \|u\|^2_{H^2(0,1)},$$

$$I_7 := c_3(|h - h_k| + |h' - h'_k|)|u_k(\tau,1)|(|w_k(1) - u(1)| + |e(1)|)$$

$$\leq c_3(|h - h_k| + |h' - h'_k|)\hat{c}\,\|u_k\|^{1-\theta}\left\|\frac{\partial u_k}{\partial y}\right\|^\theta (|w_k(1) - u(1)| + |e(1)|)$$

$$\leq c_3(|h - h_k| + |h' - h'_k|)\hat{c}^2\,\|u_k\|_{H^1(0,1)}\left(\gamma_1 k^2 + \gamma_3 k^{1+\theta}\right)\|u\|_{H^2(0,1)}$$

$$+ c_3(|h - h_k| + |h' - h'_k|)\hat{c}^2\,\|u_k\|_{H^1(0,1)}\,\|e\|^\theta\,\|e\|^{1-\theta}_{H^1(0,1)}$$

$$\leq c_3\hat{c}^2(|h - h_k| + |h' - h'_k|)\,\|u_k\|_{H^1(0,1)}\left(\gamma_1 k^2 + \gamma_3 k^{1+\theta}\right)\|u\|_{H^2(0,1)}$$

$$+ c_3\hat{c}^2(|h - h_k| + |h' - h'_k|)\,\|u_k\|_{H^1(0,1)}\,\|e\|^\theta\,\|e\|^{1-\theta}_{H^1(0,1)}$$

$$\leq \xi\,(|h - h_k| + |h' - h'_k|)^2\,\|u_k\|^2_{H^1(0,1)} + c_\xi\left(c_3\hat{c}^2(\gamma_1 k^2 + \gamma_3 k^{1+\theta})\right)^2 \|u\|^2_{H^2(0,1)}$$

$$+ \bar{\xi}\,(|h - h_k| + |h' - h'_k|)^2\,\|u_k\|^2_{H^1(0,1)} + c_{\bar{\xi}}c_3^2\hat{c}^4\|e\|^{2\theta}\,\|e\|^{2(1-\theta)}_{H^1(0,1)}$$

$$\leq 2\xi\hat{c}_1\left(|h - h_k|^2 + |h' - h'_k|^2\right) + c_\xi\left(c_3\hat{c}^2(\gamma_1 k^2 + \gamma_3 k^{1+\theta})\right)^2 \|u\|^2_{H^2(0,1)}$$

$$+ 2\bar{\xi}\hat{c}_1\left(|h - h_k|^2 + |h' - h'_k|^2\right) + \hat{\xi}\frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + \left(\frac{\hat{\xi}}{h^2} + c_{\hat{\xi}}c_{\bar{\xi}}^2 c_3^4\hat{c}^8 h^2\right)\|e\|^2,$$

$$I_8 := c_4\mathrm{Bi}\frac{b^*}{m_0}|h - h_k|\,(|w_k(0) - u(0)| + |e(0)|)$$

$$\leq c_4\mathrm{Bi}\frac{b^*}{m_0}|h - h_k|\left(\hat{c}(\gamma_1 k^2 + \gamma_3 k^{1+\theta})\,\|u\|_{H^2(0,1)} + \hat{c}\,\|e\|^\theta\,\|e\|^{1-\theta}_{H^1(0,1)}\right)$$

$$\leq \xi|h - h_k|^2 + c_\xi c_4^2\hat{c}^2\mathrm{Bi}^2\frac{(b^*)^2}{m_0^2}(\gamma_1 k^2 + \gamma_3 k^{1+\theta})^2\|u\|^2_{H^2(0,1)}$$

$$+ \hat{\xi}|h - h_k|^2 + c_{\hat{\xi}}c_4^2\hat{c}^2\mathrm{Bi}^2\frac{(b^*)^2}{m_0^2}\,\|e\|^{2\theta}\,\|e\|^{2(1-\theta)}_{H^1(0,1)}$$

$$\leq \xi|h - h_k|^2 + c_\xi c_4^2\hat{c}^2\mathrm{Bi}^2\frac{(b^*)^2}{m_0^2}(\gamma_1 k^2 + \gamma_3 k^{1+\theta})^2\|u\|^2_{H^2(0,1)}$$

$$+ \hat{\xi}|h - h_k|^2 + \bar{\xi}\frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + \left(\frac{\bar{\xi}}{h^2} + c_{\bar{\xi}}c_{\hat{\xi}}^2 c_4^4\hat{c}^4\mathrm{Bi}^4\frac{(b^*)^4}{m_0^4}h^2\right)\|e\|^2.$$

By a similar calculation used to obtain the upper bounds on I_6 and I_8, we get

$$I_9 := c_5\mathrm{Bi}\,\mathrm{H}(|e(0)| + |h - h_k|)(|w_k(0) - u(0)| + |e(0)|)$$

$$\leq \frac{3}{2}\left(\frac{\xi}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + \left(\frac{\xi}{h^2} + c_\xi \hat{c}^2 c_5^2\mathrm{Bi}^2\mathrm{H}^2 h^2\right)\|e\|^2\right)$$

$$+ c_\xi c_5^2\mathrm{Bi}^2\mathrm{H}^2\hat{c}^2(\gamma_1 k^2 + \gamma_3 k^{1+\theta})^2\,\|u\|^2_{H^2(0,1)}$$

$$+ (\xi + \hat{\xi})|h - h_k|^2 + \bar{\xi}\frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + \left(\frac{\bar{\xi}}{h^2} + c_{\bar{\xi}}c_{\hat{\xi}}^2 c_5^4\hat{c}^4\mathrm{Bi}^4\mathrm{H}^4 h^2\right)\|e\|^2.$$

Finally, we are led to the following structural inequality:

$$
(51) \qquad \frac{1}{2}\frac{d}{d\tau}\|e\|^2 + A_1 \left\|\frac{\partial e}{\partial y}\right\|^2 \le A_2 k^2 + A_3\|e\|^2 + A_4|h-h_k|^2 + A_5|h'-h_k'|^2,
$$

where

$$
A_1 := \frac{1}{L^2}\left(1 - \frac{5}{2}\xi - \hat{\rho} - \zeta - 2\hat{\xi} - 2\bar{\xi}\right),
$$

$$
A_2 := \|u\|_{H^2(0,1)}\left(\frac{\gamma_1^2}{2} + \frac{1}{h_0^2}c_\xi\gamma_2^2 + c_\rho c_1^2\gamma_2^2 + 2c_\zeta\|h'\|_\infty^2\gamma_1^2 + c_\xi c_2^2\gamma_2^2\right.
$$

$$
+ \frac{\|h'\|_\infty}{2h_0}\hat{c}^2(\gamma_1+\gamma_3)^2 + c_\xi c_3^2\hat{c}^4(\gamma_1+\gamma_3)^2 + c_\xi c_4^2\hat{c}^2\mathrm{Bi}^2\frac{(b^*)^2}{m_0^2}(\gamma_1+\gamma_3)^2
$$

$$
\left. + c_\xi c_5^2\hat{c}^2\mathrm{Bi}^2\,\mathrm{H}^2(\gamma_1+\gamma_3)^2\right),
$$

$$
A_3 := 2c_\zeta\|h'\|_\infty^2 + \frac{1}{h_0^2}\left(3\xi + \hat{\xi} + 2\bar{\xi}\right) + \frac{3}{2}c_\xi\hat{c}^2\|h'\|_\infty^2 + c_{\hat{\xi}}c_\xi^2 c_3^4\hat{c}^8\|h\|_\infty^2
$$

$$
+ c_{\bar{\xi}}c_{\hat{\xi}}^2\hat{c}^4\mathrm{Bi}^4\left(c_4^4\frac{(b^*)^4}{m_0^4} + c_5^4\mathrm{H}^4\right)\|h\|_\infty^2 + c_\xi\hat{c}^2 c_5^2\mathrm{Bi}^2\,\mathrm{H}^2\|h\|_\infty^2,
$$

$$
A_4 := 2(\xi+\hat{\xi}) + \hat{c}_1(\rho+\xi) + 2\hat{c}_1(\bar{\xi}+\xi) + c_{\hat{\rho}}\hat{c}_1 c_1^2\|h\|_\infty^2 + c_2^2\hat{c}_1 c_{\hat{\xi}}\|h\|_\infty^2,
$$

$$
A_5 := 3\xi\hat{c}_1 + 2\bar{\xi}\hat{c}_1 + c_2^2\hat{c}_1 c_{\hat{\xi}}\|h\|_\infty^2.
$$

From (19) and (23), we get for all $\tau \in (0,\hat{T})$ the inequality

$$
|h'(\tau) - h_k'(\tau)| \le A_0|e(1)| + \frac{1}{m_0}|\sigma(h(\tau)) - \sigma(h_k(\tau))|
$$

$$
\le A_0\hat{c}\left(\eta\|e(\tau)\|_{H^1(0,1)} + c_\eta\|e(\tau)\|\right) + \frac{\mathcal{L}}{m_0}|h(\tau) - h_k(\tau)|.
$$

Thus, this leads to

$$
(52) \qquad |h'-h_k'|^2 \le 3\left(A_0^2\hat{c}^2\eta^2\left\|\frac{\partial e}{\partial y}\right\|^2 + A_0^2\hat{c}^2(\eta^2+c_\eta^2)\|e\|^2 + \frac{\mathcal{L}^2}{m_0^2}|h-h_k|^2\right).
$$

Using (52) in (51), we infer that

(53)
$$
\frac{d}{d\tau}\|e\|^2 + (A_1 - 3A_0^2\hat{c}^2\eta^2 A_5)\left\|\frac{\partial e}{\partial y}\right\|^2 \le A_2 k^2 + A_6\|e\|^2 + \left(A_4 + 3A_5\frac{\mathcal{L}^2}{m_0^2}\right)|h-h_k|^2,
$$

where $A_6 := A_3 + 3A_0^2\hat{c}^2(\eta^2+c_\eta^2)A_5$. We choose $\xi > 0$, $\hat{\rho} > 0$, $\bar{\xi} > 0$, $\zeta > 0$, $\hat{\xi} > 0$, and $\eta > 0$ sufficiently small such that $\zeta_1 := A_1 - 3A_0^2\hat{c}^2\eta^2 A_5 > 0$. Applying Gronwall's inequality (see e.g. Appendix B in [7]) gives the following upper bounds:

$$
\|e(\tau)\|^2 \le e^{\int_0^\tau A_6 ds}\left(\|e(0)\|^2 + \int_0^\tau\left(A_2 k^2 + \left(A_4 + 3A_5\frac{\mathcal{L}^2}{m_0^2}\right)|h(s)-h_k(s)|^2\right)ds\right)
$$

$$
\le c_6(A_0,A_3,A_5,\hat{T})\left(k^4\|u_0\|_{H^2(0,1)}^2 + A_2 k^2\tau\right.
$$

$$
+ \left.\left(A_4 + 3A_5\frac{\mathcal{L}^2}{m_0^2}\right)\int_0^\tau|h(s)-h_k(s)|^2 ds\right)
$$

$$
\le c_6(A_0,A_3,A_4,A_5,\mathcal{L},\hat{T})\left(k^4 + k^2\hat{T} + \|h-h_k\|_{L^2(S_{\hat{T}})}^2\right).
$$

Thus, we obtain

$$\max_{0 \le \tau \le \hat{T}} \|e(\tau)\|^2 \le c_6 \left(k^2 + \|h - h_k\|^2_{L^2(S_{\hat{T}})} \right).$$

By using Young's inequality together with (52), we get the following relations:

$$\frac{d}{d\tau}(|h - h_k|^2) = 2(h - h_k)(h' - h_k')$$
$$\le |h - h_k|^2 + |h' - h_k'|^2$$

$$(54) \qquad \le C|h - h_k|^2 + 3A_0^2 \hat{c}^2 \eta^2 \left\| \frac{\partial e}{\partial y} \right\|^2 + 3A_0^2 \hat{c}^2 (\eta^2 + c_\eta^2) \|e\|^2,$$

where $C := 1 + 3\mathcal{L}^2/m_0^2$.

Let $\delta > 0$ be any positive real number. Adding $\delta \frac{d}{d\tau} |h - h_k|^2$ on both sides of (53) and using (54) yields

$$\frac{d}{d\tau} \left(\|e\|^2 + \delta|h - h_k|^2 \right) + (\zeta_1 - 3\delta \hat{c}^2 A_0^2 \eta^2) \left\| \frac{\partial e}{\partial y} \right\|^2$$
$$\le A_2 k^2 + (A_6 + 3\delta A_0^2 \hat{c}^2 (\eta^2 + c_\eta^2)) \|e\|^2$$
$$+ \left(A_4 + 3A_5 \frac{\mathcal{L}^2}{m_0^2} + \delta C \right) |h - h_k|^2.$$

We choose $\eta > 0$ in such a way that $(\zeta_1 - 3\delta \hat{c}^2 A_0^2 \eta^2) > 0$. Then it exists a constant $A_7 > 0$ such that

$$(55) \qquad \frac{d}{d\tau} \left(\|e\|^2 + \delta|h - h_k|^2 \right) \le A_2 k^2 + A_7 (\|e\|^2 + \delta|h - h_k|^2).$$

Gronwall's inequality applied to (55) for the quantity $\|e\|^2 + \delta|h - h_k|^2$ gives the estimate

$$(56) \qquad \|e\|^2 + \delta|h - h_k|^2 \le ck^2.$$

Integrating (53) from 0 to $\hat{T}$ and using (56) yields

$$(57) \qquad \int_0^{\hat{T}} \left\| \frac{\partial e}{\partial y} \right\|^2 d\tau \le c_7 k^2.$$

Integrating (52) from 0 to $\hat{T}$ and using (56) and (57) gives the estimate

$$\|h' - h_k'\|^2 \le ck^2,$$

which completes the proof of Theorem 5.1. □

Theorem 5.2. *(A posteriori error estimate) Assume* (A1)–(A5) *hold. Additionally, take* $u_0 \in H^2(0,1)$. *Let* (u, h) *and* (u_k, h_k) *be the corresponding weak solutions to the problem* (P) *and* (P_d) *in the sense of Definition 4.1 and Definition 4.2, respectively. Then there exist* $0 < \tilde{T} \le \hat{T}$ *and positive constants* c_1, c_2, c_3 *(independent of* k *and* u*) such that for all* $\tau \in S_{\tilde{T}} := (0, \tilde{T})$ *the following inequality holds:*

$$\|u - u_k\|_{L^2(0,1)} + c_1|h - h_k|^2 + c_2 \int_0^\tau \left\| \frac{\partial}{\partial x}(u - u_k) \right\|^2 ds$$

$$(58) \qquad \le c_3 \left(|h(0) - h_k(0)|^2 + \sum_{i=0}^{N-2} k_i^2 \left\{ \|R(u_k)\|^2_{L^2(S_{\tilde{T}}, L^2(I_i))} + k_i^2 \|u_0\|^2_{H^2(I_i)} \right\} \right),$$

where the residual $R(u_k)$ is defined by

$$(59) \qquad R(u_k) := \frac{h'_k}{h_k} y \frac{\partial u_k}{\partial y} + \frac{1}{h_k} \text{Bi} \left(\frac{b(\tau)}{m_0} - \text{H} u_k(\tau, 0) \right) - \frac{h'_k}{h_k} u_k(\tau, 1) - \frac{\partial u_k}{\partial \tau}.$$

Proof. Let $e := u - u_k$ be the pointwise error. Using the weak formulation (18), we can write

$$
\begin{aligned}
\left(\frac{\partial e}{\partial \tau}, v \right) + \frac{1}{h^2} \left(\frac{\partial e}{\partial y}, \frac{\partial v}{\partial y} \right) &= \left[\left(\frac{\partial u}{\partial \tau}, v \right) + \frac{1}{h^2} \left(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y} \right) \right] \\
&\quad - \left[\left(\frac{\partial u_k}{\partial \tau}, v \right) + \frac{1}{h^2} \left(\frac{\partial u_k}{\partial y}, \frac{\partial v}{\partial y} \right) \right] \\
&= \frac{h'}{h} \int_0^1 y \frac{\partial u}{\partial y} v \, dy + \frac{1}{h} \text{Bi} \left(\frac{b(\tau)}{m_0} - \text{H} u(\tau, 0) \right) v(0) \\
&\quad - \frac{h'}{h} u(\tau, 1) v(1) - \left[\left(\frac{\partial u_k}{\partial \tau}, v \right) + \frac{1}{h_k^2} \left(\frac{\partial u_k}{\partial y}, \frac{\partial v}{\partial y} \right) \right. \\
(60) &\quad \left. + \left(\frac{1}{h^2} - \frac{1}{h_k^2} \right) \left(\frac{\partial u_k}{\partial y}, \frac{\partial v}{\partial y} \right) \right]
\end{aligned}
$$

for all $v \in H^1(0, 1)$. Inserting (59) into (60) yields

$$
\begin{aligned}
\left(\frac{\partial e}{\partial \tau}, v \right) + \frac{1}{h^2} \left(\frac{\partial e}{\partial y}, \frac{\partial v}{\partial y} \right) &= \frac{h'}{h} \int_0^1 y \frac{\partial u}{\partial y} v \, dy + \frac{1}{h} \text{Bi} \left(\frac{b(\tau)}{m_0} - \text{H} u(\tau, 0) \right) v(0) \\
&\quad - \frac{h'}{h} u(\tau, 1) v(1) - \left(\frac{1}{h^2} - \frac{1}{h_k^2} \right) \left(\frac{\partial u_k}{\partial y}, \frac{\partial v}{\partial y} \right) \\
&\quad - \frac{h'_k}{h_k} \int_0^1 y \frac{\partial u_k}{\partial y} v \, dy - \frac{1}{h_k} \text{Bi} \left(\frac{b(\tau)}{m_0} - \text{H} u_k(\tau, 0) \right) v(0) \\
(61) &\quad + \frac{h'_k}{h_k} u_k(\tau, 1) v(1) + \left[\int_0^1 R(u_k) v \, dy - \frac{1}{h_k^2} \left(\frac{\partial u_k}{\partial y}, \frac{\partial v}{\partial y} \right) \right],
\end{aligned}
$$

where $R(u_k)$ is the residual quantity defined in (59). Since $u_k \in V_k$, we have that $\frac{\partial^2 u_k}{\partial y^2} = 0$ on each $I_i := (y_i, y_{i+1})$. The term

$$\int_0^1 R(u_k) v \, dy - \frac{1}{h_k^2} \left(\frac{\partial u_k}{\partial y}, \frac{\partial v}{\partial y} \right)$$

becomes after integration by part

$$\sum_{i=0}^{N-2} \left\{ \int_{y_i}^{y_{i+1}} R(u_k) v \, dy - \frac{1}{h_k^2} \left(\frac{\partial u_k}{\partial y}(y_{i+1}) v(y_{i+1}) - \frac{\partial u_k}{\partial y}(y_i) v(y_i) \right) \right\}.$$

We also get from (22)

$$(62) \quad \sum_{i=0}^{N-2} \left\{ \int_{y_i}^{y_{i+1}} R(u_k) v_k \, dy - \frac{1}{h_k^2} \left(\frac{\partial u_k}{\partial y}(y_{i+1}) v_k(y_{i+1}) - \frac{\partial u_k}{\partial y}(y_i) v_k(y_i) \right) \right\} = 0$$

for all $v_k \in V_k$. Adding (62) to (61) while taking $v = e \in H^1(0, 1)$ and $v_k = I_k e \in V_k$ gives

$$\frac{1}{2} \frac{d}{d\tau} \|e\|^2 + \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 = \frac{h'}{h} \int_0^1 y \frac{\partial u}{\partial y} e \, dy + \frac{1}{h} \text{Bi} \left(\frac{b(\tau)}{m_0} - \text{H} u(\tau, 0) \right) e(0)$$

$$- \frac{h'}{h} u(\tau,1) e(1) - \left(\frac{1}{h^2} - \frac{1}{h_k^2} \right) \left(\frac{\partial u_k}{\partial y}, \frac{\partial e}{\partial y} \right) - \frac{h_k'}{h_k} \int_0^1 y \frac{\partial u_k}{\partial y} e \, dy$$

$$- \frac{1}{h_k} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} - \mathrm{H} u_k(\tau,0) \right) e(0) + \frac{h_k'}{h_k} u_k(\tau,1) e(1)$$

$$+ \sum_{i=0}^{N-2} \left\{ \int_{y_i}^{y_{i+1}} R(u_k)(e - I_k e) \, dy \right.$$

$$\left. - \frac{1}{h_k^2} \left(\frac{\partial u_k}{\partial y}(y_{i+1})(e - I_k e)(y_{i+1}) - \frac{\partial u_k}{\partial y}(y_i)(e - I_k e)(y_i) \right) \right\}$$

$$= \sum_{i=1}^{5} I_i,$$

where

$$I_1 := \frac{h'}{h} \int_0^1 y \frac{\partial u}{\partial y} e \, dy - \frac{h_k'}{h_k} \int_0^1 y \frac{\partial u_k}{\partial y} e \, dy,$$

$$I_2 := \frac{1}{h} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} - \mathrm{H} u(\tau,0) \right) e(0) - \frac{1}{h_k} \mathrm{Bi} \left(\frac{b(\tau)}{m_0} - \mathrm{H} u_k(\tau,0) \right) e(0),$$

$$I_3 := \frac{h_k'}{h_k} u_k(\tau,1) e(1) - \frac{h'}{h} u(\tau,1) e(1),$$

$$I_4 := - \left(\frac{1}{h^2} - \frac{1}{h_k^2} \right) \left(\frac{\partial u_k}{\partial y}, \frac{\partial e}{\partial y} \right),$$

$$I_5 := \sum_{i=0}^{N-2} \left\{ \int_{y_i}^{y_{i+1}} R(u_k)(e - I_k e) \, dy \right.$$

$$\left. - \frac{1}{h_k^2} \left(\frac{\partial u_k}{\partial y}(y_{i+1})(e - I_k e)(y_{i+1}) - \frac{\partial u_k}{\partial y}(y_i)(e - I_k e)(y_i) \right) \right\}.$$

By using (26) together with Cauchy-Schwarz and Young's inequality, we obtain

$$|I_1| \leq \frac{h'}{h} \left\| \frac{\partial e}{\partial y} \right\| \|e\| + \left| \frac{h'}{h} - \frac{h_k'}{h_k} \right| \|e\|$$

$$(63) \quad \leq \left(\frac{\xi}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 + c_\xi \|h'\|_\infty^2 \|e\|^2 \right) + \xi \|e\|^2 + 2 c_\xi \left(|h - h_k|^2 + |h' - h_k'|^2 \right).$$

$$|I_2| \leq \mathrm{Bi} \frac{b(\tau)}{m_0} \frac{1}{h h_k} |h - h_k| |e(0)| + \mathrm{Bi} \, \mathrm{H} \left| \frac{u(\tau,0)}{h} - \frac{u_k(\tau,0)}{h_k} \right| |e(0)|$$

$$\leq \left(\mathrm{Bi} \frac{b^*}{m_0} \frac{1}{L^2} \hat{c} + \mathrm{Bi} \, \mathrm{H} \hat{c} \right) |h - h_k| \|e\|^{1-\theta} \left\| \frac{\partial e}{\partial y} \right\|^\theta + c_2 \mathrm{Bi} \, \mathrm{H} \hat{c} \|e\|^{2(1-\theta)} \left\| \frac{\partial e}{\partial y} \right\|^{2\theta}$$

$$(64) \quad \leq \bar{\xi} |h - h_k|^2 + \xi c_{\bar{\xi}} \frac{1}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 + \tilde{c}^4 c_\xi c_{\bar{\xi}} h^2 \|e\|^2 + \frac{\xi}{h^2} \left\| \frac{\partial e}{\partial y} \right\|^2 + \tilde{c}_1^2 c_\xi h^2 \|e\|^2,$$

where

$$\theta = \frac{1}{2}, \quad \tilde{c} := \left(\mathrm{Bi} \frac{b^*}{m_0} \frac{1}{L^2} \hat{c} + \mathrm{Bi} \, \mathrm{H} \hat{c} \right) \quad \text{and} \quad \tilde{c}_1 := c_2 \mathrm{Bi} \, \mathrm{H} \hat{c}.$$

$$|I_3| \leq \left| \frac{h'}{h} - \frac{h_k'}{h_k} \right| |e(1)| + \frac{h_k'}{h_k} |e(1)|^2$$

$$\leq 2\bar{\xi}\left(|h-h_k|^2 + |h'-h_k'|^2\right) + \xi\frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2$$

$$(65) \qquad + c_{\bar{\xi}}c_\xi c_3^4 \hat{c}^4 \|e\|^2 h^2 + c\left(\frac{\xi}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + c_\xi\|e\|^2\right).$$

$$|I_4| \leq |h-h_k|\frac{h+h_k}{h^2 h_k^2}\left\|\frac{\partial u_k}{\partial y}\right\|\left\|\frac{\partial e}{\partial y}\right\|$$

$$(66) \qquad \leq \xi|h-h_k|^2 + c_\xi c^2(h_0, L)\frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2.$$

To bound $|I_5|$ from above, we use the fact that $I_k e$ is the Lagrange interpolant of e with the property $(e - I_k e)(y_i) = 0$, $i \in \{0, 1, 2, \cdots, N-1\}$. We have

$$|I_5| \leq \sum_{i=0}^{N-2} \int_{y_i}^{y_{i+1}} R(u_k)(e - I_k e)dy$$

$$\leq \sum_{i=0}^{N-2} \|R(u_k)\|_{L^2(I_i)}\|e - I_k e\|_{L^2(I_i)}$$

$$\leq \tilde{c}\sum_{i=0}^{N-2} \|R(u_k)\|_{L^2(I_i)}k_i\left\|\frac{\partial e}{\partial y}\right\|_{L^2(I_i)}$$

$$\leq \tilde{c}\left(\sum_{i=0}^{N-2}\|R(u_k)\|_{L^2(I_i)}^2 k_i^2\right)^{\frac{1}{2}}\left(\sum_{i=0}^{N-2}\left\|\frac{\partial e}{\partial y}\right\|_{L^2(I_i)}^2\right)^{\frac{1}{2}}$$

$$= \tilde{c}\left(\sum_{i=0}^{N-2}\|R(u_k)\|_{L^2(I_i)}^2 k_i^2\right)^{\frac{1}{2}}\left\|\frac{\partial e}{\partial y}\right\|_{L^2(0,1)}.$$

By using Young's inequality, we obtain

$$(67) \qquad |I_5| \leq \frac{\xi}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 + c_\xi \tilde{c}^2 h^2 \sum_{i=0}^{N-2}\|R(u_k)\|_{L^2(I_i)}^2 k_i^2.$$

It follows from (63)–(67) that for all ξ, $\bar{\xi} > 0$, there exist positive constants K_1, K_2, K_3 and K_4 such that

$$\frac{1}{2}\frac{d}{d\tau}\|e\|^2 + \frac{1}{h^2}\left\|\frac{\partial e}{\partial y}\right\|^2 \leq K_1\|e\|^2 + K_2|h-h_k|^2$$

$$+ \frac{1}{h^2}K_3\left\|\frac{\partial e}{\partial y}\right\|^2 + K_4\sum_{i=0}^{N-2}\|R(u_k)\|_{L^2(I_i)}^2 k_i^2.$$

Let $\delta > 0$ be a fixed, sufficiently small. Adding $\frac{\delta}{2}\frac{d}{d\tau}|h-h_k|^2$ on both sides and using (54) yields

$$\frac{1}{2}\frac{d}{d\tau}\left(\|e\|^2 + \delta|h-h_k|^2\right) + \frac{1}{L^2}(1 - K_3 - 3\delta A_0^2\eta)\left\|\frac{\partial e}{\partial y}\right\|^2$$

$$\leq K_1\|e\|^2 + K_2|h-h_k|^2 + 3\delta A_0^2 c_\eta\|e\|^2 + C\delta|h-h_k|^2 + K_4\sum_{i=0}^{N-2}\|R(u_k)\|_{L^2(I_i)}^2 k_i^2.$$

We choose $\xi > 0$, $\bar{\xi} > 0$ and $\eta > 0$ in such a way that $1 - K_3 - 3\delta A_0^2\eta \geq 0$. Then it exists $K_5 > 0$ such that

$$\frac{1}{2}\frac{d}{d\tau}\left(\|e\|^2 + \delta|h - h_k|^2\right) + \frac{1}{L^2}(1 - K_3 - 3\delta A_0^2 \eta)\left\|\frac{\partial e}{\partial y}\right\|^2$$

(68)
$$\leq K_5(\|e\|^2 + \delta|h - h_k|^2) + K_4 \sum_{i=0}^{N-2} \|R(u_k)\|_{L^2(I_i)}^2 k_i^2.$$

Applying Gronwall's inequality to (68) for the quantity $\|e\|^2 + \delta|h - h_k|^2$ and using the initial condition

$$\|e(0)\|_{L^2(0,1)}^2 = \sum_{i=0}^{N-2} \|e(0)\|_{L^2(I_i)}^2 \leq k_i^4 \|u_0\|_{H^2(I_i)}^2,$$

it exists a constant $c(\tilde{T}, L)$ such that

$$\|e\|^2 + \delta|h(\tau) - h_k(\tau)|^2 \leq c(\tilde{T}, L)\left(|h(0) - h_k(0)|^2 + k_i^4\|u_0\|_{H^2(I_i)}^2\right.$$

(69)
$$\left. + \sum_{i=0}^{N-2}\int_0^\tau \|R(u_k)\|_{L^2(I_i)}^2 k_i^2 ds\right).$$

By integrating (68) on $(0, \tau)$ and by using (69), it exists another constant $c(\tilde{T}, L) > 0$ such that the following inequality holds:

$$\int_0^\tau \left\|\frac{\partial}{\partial x}(u - u_k)\right\|^2 ds \leq c(\tilde{T}, L)\left(|h(0) - h_k(0)|^2 + k_i^4\|u_0\|_{H^2(I_i)}^2\right.$$

$$\left. + \sum_{i=0}^{N-2}\int_0^\tau \|R(u_k)\|_{L^2(I_i)}^2 k_i^2 ds\right).$$

This concludes the proof of Theorem 5.2. □

6. Numerical illustrations

In this section, we firstly present our simulation results for both the dense and foam rubber. The difference in the two cases is incorporated in the choice of parameters. To approximate numerically the weak solution to (22)–(25), we use the method of lines; for more details see, for instance, [2]. Firstly, the model equations are discretized in space by means of the finite element method. The resulting time-dependent system of ordinary differential equations is tackled via the solver `odeint` in Python; see [20] for details on Python and [12] for details on the solver. We refer the reader to see our previous work [1] for the laboratory experiments, numerical method and simulation results where we investigated the parameter space by exploring eventual effects of the choice of parameters on the overall diffusants penetration process.

We take as observation time $T_f = 40$ minutes for the final time with time step $\Delta t = 1/1000$ minutes. We choose the number of space discretization points N to be 100. The values of parameters are taken to be $s_0 = 0.01$ (mm), $m_0 = 0.1$ (gram/mm^3) and $b = 1$ (gram/mm^3). We take the value 3.66×10^{-4} (mm^2/min) for the diffusion constant D [14], 0.564 (mm/min) for absorption rate β [15] and 2.5 for Henry's constant H [13]. For the dense rubber, we choose $\sigma(s(t)) = s(t)/10$ (gram/mm^3) and $a_0 = 500$ (mm^4/sec/gram) while we choose $\sigma(s(t)) = s(t)/50$ (gram/mm^3) and $a_0 = 2000$ (mm^4/sec/gram) for the foam rubber case.
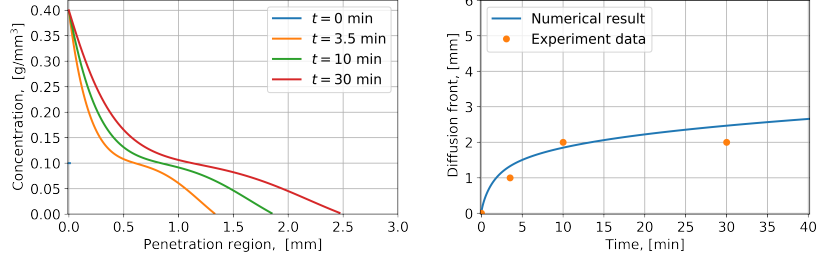
FIGURE 2. Dense rubber case. Left: Concentration profile of diffusant. Right: Position of the moving boundary.
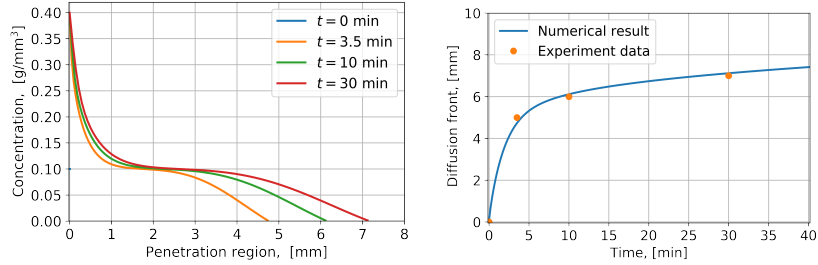

FIGURE 3. Foam rubber case. Left: Concentration profile of diffusants. Right: Position of the moving boundary.

In Figure 2 and Figure 3 we show the concentration profile of the penetrating diffusant, and respectively, the position of the moving boundary for the dense rubber and foam rubber respectively. Comparing the diffusant concentration profile in Figure 2 and Figure 3, we notice in both cases that, within a short time of release of diffusant from its initial position, the diffusant quickly enters the rubber from the left boundary and then starts diffusing inside displacing a penetration front. In bothe Figure 2 and Figure 3, we compare simulation results against experimental data for the position of moving boundary. Both plots show a good agreement between model and experiment.

Finally, we wish to point out that the order of convergence of our FEM scheme is consistent with the estimates stated in (46). As we are not aware of an exact solution to (22)–(25), we compute the finite element approximation of our weak solution on a fine mesh (say, with 640 nodes) and denote it by $u_{\tilde{k}}$. We use this $u_{\tilde{k}}$ as the reference solution for computing the errors and convergence orders. We make use of the discrete $\ell^2(Q(\hat{T}))$ norm which we denote here as $e(k_i) :=$

$$\left\| u_{\tilde{k}}(\tau, y) - u_{k_i}(\tau, y) \right\|_{L^2(S_{\hat{T}}, L^2(0,1))} = \left(\Delta\tau k_i \sum_{j=0}^{N_t} \sum_{\ell=0}^{N-1} |u_{\tilde{k}}(\tau_j, y_\ell) - u_{k_i}(\tau_j, y_\ell)|^2 \right)^{\frac{1}{2}}.$$

Here $\Delta\tau$ is the uniform size of the $N_t + 1$ time steps, while $\{k_1, k_2, k_3, \cdots\}$ with $k_i > k_{i+1}$ for $i \in \{1, 2, \cdots\}$ is a finite collection of the different mesh sizes used in the computations.

We determine the convergence order based on any two consecutive calculations of discrete errors using two different mesh sizes. To this end, we perform the

computations on a sequence of grids with mesh size k that are halved in each step. Thus, we use the following formula to compute the convergence order r:

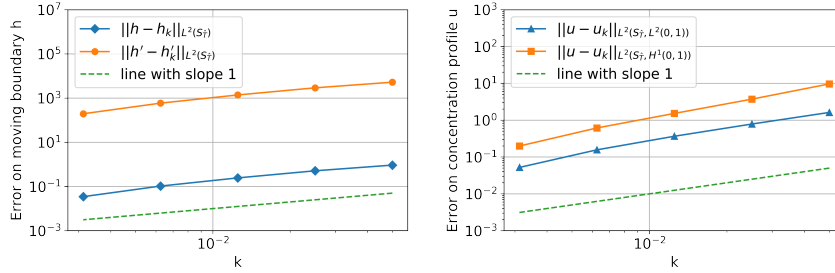$$r := \log_2 \left(\frac{e(k_i)}{e(k_{i+1})} \right).$$

FIGURE 4. Convergence order when time step size $\Delta t = 10^{-4}$ is fixed. Dash lines are lines of slope 1. Left: Log log scale plot of error on the boundary $\|h - h_k\|_{L^2(S_{\hat{T}})}$ (circles) and $\|h' - h'_k\|_{L^2(S_{\hat{T}})}$ (diamonds). Right: Log log scale plot of error on the concentration $\|u - u_k\|_{L^2(S_{\hat{T}}, L^2(0,1))}$ (triangles) and $\|u - u_k\|_{L^2(S_{\hat{T}}, H^1(0,1))}$ (squares).

We show in Figure 4 the computed convergence order for the approximation of the moving boundary position and of the concentration profile. This is done in various norms for $N = 20, 40, 80, 160$, and 320. These numerical results are in agreement with the convergence order proven in Section 5.

7. Conclusion

The goal of this work was to analyze the errors produced by a semi-discrete finite element approximation of the weak solution of moving boundary problem modeling the penetration of diffusants into rubber. We obtained the *a priori* error estimate (46) for the diffusant concentration profile as well as for the position and speed of the moving boundary. The convergence rate is of order of $\mathcal{O}(1)$ – the deviation from optimality is due to the nonlinear coupling produced by the presence of the unknown moving boundary. Additionally, we obtained the *a posteriori* error (58). Finally, we illustrated numerically the basic output of our model. It turns out that results are in the expected experimental range and they can be obtained in practice using convergence rates closed to the theoretical ones.

Acknowledgements

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