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ON A PRIORI ERROR ESTIMATES FOR A TWO-PHASE MOVING-INTERFACE PROBLEM WITH KINETIC CONDITION

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ABSTRACT. We discuss the error analysis for a moving-boundary system in two phases arising from modeling the penetration of a sharp carbonation front into unsaturated cement-based materials. The special feature of this problem is that the moving boundary is driven by a kinetic condition proportional to the rate of a fast carbonation reaction concentrated on the moving boundary. We prove *a priori* error estimates for the concentration profiles and position of the moving boundary.

1. **Introduction.** A natural way to describe fast reaction-slow transport scenarios in porous media is to employ a so-called *moving-interface model*. Such a model consists of a system of mass-balance equations whose main feature is that it describes a chemical reaction concentrated at the moving interface (or, following the case, near a thin layer, or within one or multiple larger strips [10]). Typically, the position of the moving reaction locus is *a priori* unknown. Therefore, this needs to be determined simultaneously together with the concentration profiles of the involved chemical species.

Mathematically, the moving-inteface models are interesting from at least two perspectives: they are quite difficult to classify and there is no general framework for the study of their well-posedness or numerical approximation. Usually, each model has its own particularities, and therefore, it requires specific investigation techniques. Note that, in general, one distinguishes in principle between two different classes of moving-interface models. Following the terminology from Visintin's book on modeling phase transitions [18], we have

- (A) Models with equilibrium conditions at the moving interface;
- (B) Models with non-equilibrium conditions at the moving interface.

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Free-boundary problems like those due to Stefan, Hele-Shaw, Muskat, Mullins and Sekerka belong to class (A), while moving-interface models with kinetic¹ condition belong to class (B).

In this note, we focus on a PDE model belonging to the class (B). More precisely, we deal with a moving-interface model with kinetic condition arising in the modeling of concrete carbonation. CO₂ and humidity attack concrete samples and reduce their protection to corrosion (i.e. the alkalinity) via the apparently harmless reaction $\text{CO}_2(\text{g} \rightarrow \text{aq}) + \text{Ca}(\text{OH})_2(\text{s} \rightarrow \text{aq}) \rightarrow \text{CaCO}_3 + \text{H}_2\text{O}$; see [6] for details on the physics and chemistry of the full process and [7] for a well-posedness study of a moving sharp-interface model for concrete carbonation. Note that the book by Ortoleva [15] contains a wealth of reaction-diffusion scenarios from geo-chemistry that belong to the class (B). We also draw the reader's attention to the paper [14], where a moving-boundary model with kinetic condition describing the dissolution and precipitation of salts in porous media is analyzed.

The main objective here is to extend the results of our paper [9], obtained for the case of a one-phase moving-boundary system, in two different directions. On one hand, the PDE system we have now in view is more complex (two more PDEs have been supplemented to describe the humidity behaviour in concrete, and additionally, a PDE model replaces the former ODE model for Ca(OH)₂ dissolution). On the other hand, the reaction-diffusion scenario in section 3 includes two moving phases instead of a single one. At the technical level, our approach remotely resembles [1, 12, 13], e.g., and goes in the same spirit as the works on the numerical analysis of the one-dimensional Stefan problem by A. K. Pani and collaborators; see [16, 3] and references cited therein. In what our problem concerns, we rely on previously obtained analysis results: We extensively use the positivity, L^∞ - and the energy estimates derived in [7] for the continuous case (with two moving phases) and similar estimates stated in [9] (Theorem 4.5) for the space-discrete case (with one moving phase). Herein, we enumerate a set of *a priori* error estimates that can be derived for this type of problem and give a sketch of the main ideas of the proof. In a forthcoming publication, we will complement these results with *a posteriori* estimates and use this information for an implementation of the full carbonation model in the adaptive FEM environment ALBERTA [17].

The note is organized as follows: The governing equations for the physical situation outlined above are given within a fixed-boundary formulation together with initial, boundary and interface conditions in section 3. In the same section, we also give the weak formulation and state the main result (see Theorem 3.3) – *a priori* error estimates for concentrations and interface position. Section 4 contains the main ideas of the proof.

2. Notation. The sets $\{1, 2, 5\}$ and $\{3, 6\}$ are denoted by \mathcal{I}_1 and \mathcal{I}_2 , while $\mathcal{I} := \mathcal{I}_1 \cup \{4\} \cup \mathcal{I}_2$. As a rule if $i \in \mathcal{I}_1$, then $]a, b[:=]0, 1[$; if $i \in \mathcal{I}_2$, then $]a, b[:=]1, 2[$. Let $S_T :=]0, T[$ ($T > 0$) be the time interval under consideration and $s(t)$ be the interface position at time $t \in S_T$. Here $\Omega_1(t) :=]0, s(t)[$ and $\Omega_2(t) :=]s(t), L[$ ($L > 0$)

¹The word *kinetic* means here that an explicit expression of the normal component of the velocity of the moving interface (where the bulk of the carbonation reaction is concentrated) is given as a function of the carbonation-reaction rate. Kinetic conditions have been originally introduced to describe non-equilibrium interface kinetics during rapid solidification (see e.g. [18]), where deviations from the local equilibrium occur at a rapidly moving solid-liquid interface. This is a typical situation where phase diagram information cannot describe in an accurate manner the thermodynamics at the moving interface.

are spatial domains referring to the reacted and resp. to the unreacted phase. They are mapped via Landau transformations [5, 7] into the intervals $]0, 1[$ and $]1, 2[$. u is the vector of concentrations. For concrete carbonation, we consider as active chemical species the following: In $\Omega_1(t)$, we have $u_1 := [\text{CO}_2(\text{aq})]$, $u_2 := [\text{CO}_2(\text{g})]$, $u_4 := [\text{CaCO}_3]$, and $u_5 := [\text{moisture}]$, while in $\Omega_2(t)$, we have $u_3 := [\text{Ca}(\text{OH})_2(\text{aq})]$ and $u_6 := [\text{moisture}]$. Various function spaces are used here. We only mention the Gelfand's triple $(\mathbb{V}, \mathbb{H}, \mathbb{V}^*)$, where $\mathbb{H} := L^2(0, 1)^{|\mathcal{I}_1|} \times L^2(1, 2)^{|\mathcal{I}_2|}$ and $\mathbb{V} := \prod_{i \in \mathcal{I}-4} V_i$, while $V_i := \{w \in H^1(0, 1) : w(0) = 0\}$ for $i \in \mathcal{I}_1$ and $V_i := H^1(1, 2)$ for $i \in \mathcal{I}_2$. Furthermore, the set $W_2^1(S_T, \mathbb{V}, \mathbb{H}) := \{w \in L^2(S_T, \mathbb{V}) \text{ and } w_t \in L^2(S_T, \mathbb{V}^*)\}$ is a Banach space with the norm

$$\|w\|_{W_2^1} := \|w\|_{L^2(S_T, \mathbb{V})} + \|w'\|_{L^2(S_T, \mathbb{V}^*)}.$$

For details on the other involved Lebesgue, Sobolev and Bochner spaces, we refer the reader to [19].

3. PDE model with moving interface, weak formulation and main result.

In a fixed-domain formulation, the problem reads: Find the couple $(u(y, t), s(t))$ ($y \in]a, b[, t \in S_T$) satisfying the following system of partly dissipative PDEs:

$$(u_1 + \lambda_1)_t - \frac{D_1}{s^2} u_{1,yy} = -P_1(u_1 - Q_1 u_2) + y \frac{s'}{s} u_{1,y} \text{ in }]0, 1[, \quad (1)$$

$$(u_2 + \lambda_2)_t - \frac{D_2}{s^2} u_{2,yy} = P_2(u_1 - Q_2 u_2) + y \frac{s'}{s} u_{2,y} \text{ in }]0, 1[, \quad (2)$$

$$(u_3 + \lambda_3)_t - \frac{D_3}{(L-s)^2} u_{3,yy} = -S_{3,diss}(u_3 - u_{3,eq}) + (2-y) \frac{s'}{L-s} u_{2,y} \text{ in }]1, 2[, \quad (3)$$

$$u_4'(t) = \eta_\Gamma(u(s(t), t)), \text{ for all } t \in S_T, \quad (4)$$

$$(u_5 + \lambda_5)_t - \frac{D_5}{s^2} u_{5,yy} = y \frac{s'}{s} u_{5,y} \text{ in }]0, 1[, \quad (5)$$

$$(u_6 + \lambda_6)_t - \frac{D_6}{(L-s)^2} u_{6,yy} = (2-y) \frac{s'}{L-s} u_{2,y} \text{ in }]1, 2[, \quad (6)$$

with boundary conditions

$$u_1(0, t) = u_2(0, t) = u_{3,y}(2, t) = u_5(0, t) = u_{6,y}(0, t) = 0, \quad (7)$$

moving interface conditions

$$-\frac{D_1}{s} = \eta_\Gamma(1) + s'(u_1(1) + \lambda_1), \quad (8)$$

$$-\frac{D_2}{s} = s'(u_2(1) + \lambda_2), \quad (9)$$

$$-\frac{D_3}{L-s} = -\eta_\Gamma(1, t) + s'(u_3(1) + \lambda_3), \quad (10)$$

$$\frac{-D_5}{s} = -\frac{D_6}{L-s} - \eta_\Gamma(1, t), \quad u_5(1) + \lambda_5 = u_6(1) + \lambda_6, \quad (11)$$

as well as homogeneous initial conditions. The PDE system is closed by the kinetic condition

$$s'(t) = \eta_\Gamma(1, t) \text{ for all } t \in S_T. \quad (12)$$

The original PDE model can be obtained by transforming (1)–(12) backwards to the moving domains via inverse Landau transformation [5, 8]. Note that in the original domain the reaction rate has the form $\eta_\Gamma(u(s(t), t), t)$ for all $t \in S_T$, while $\eta_\Gamma(1, t)$

is a notation valid in the fixed-domain formulation. In what will follow, we refer to (1)–(12) as problem P_Γ and to its semi-discrete counterpart as problem P_Γ^{sd} .

Definition 3.1. The couple (u, s) is called weak solution of problem P_Γ if and only if there is $S_\delta :=]0, \delta[$ with $\delta \in]0, T[$ such that

$$s_0 < s(\delta) \leq L_0 < L, \quad (13)$$

$$u \in W_2^1(S_\delta; \mathbb{V}, \mathbb{H}) \cap [\bar{S}_\delta \rightarrow L^\infty(a, b)]^{|\mathcal{I}|}, \quad s \in W^{1,4}(S_\delta), \quad (14)$$

$$\begin{aligned} & s \sum_{i \in \mathcal{I}_1} (u_{i,t}(t), \varphi_i) + (L - s) \sum_{i \in \mathcal{I}_2} (u_{i,t}(t), \varphi_i) + A(s, u, \varphi) + E(s', u + \lambda, \varphi) \\ &= B_F(u + \lambda, s, \varphi) + H(s', u, \varphi) - s \sum_{i \in \mathcal{I}} (u_{i,t}(t), \varphi_i), \text{ and } u'_4(t) = \eta_\Gamma(u(s(t), t), \end{aligned} \quad (15)$$

$$s'(t) = \eta_\Gamma(1, t), \quad (16)$$

for all $\varphi \in \mathbb{V}$ a.e. $t \in S_\delta$ and

$$u(0) = u_0 \in \mathbb{H}, s(0) = s_0 > 0. \quad (17)$$

The expressions of $A(\cdot), E(\cdot), B_F(\cdot)$, and $H(\cdot)$ can be obtained easily by writing down the weak formulation of (1)–(12) and identifying respectively the transport term by diffusion, the boundary terms, the forcing terms as well as the new terms arising due to the immobilization of the moving interface.

Definition 3.2. The couple (u_h, s_h) is called weak solution of problem P_Γ^{sd} if and only if there is $S_\theta :=]0, \theta[$ with $\theta \in]0, T[$ such that

$$s_0 < s_h(\theta) \leq L_0 < L, \quad (18)$$

$$u_h \in W_2^1(S_\theta; \mathbb{V}_h, \mathbb{H}) \cap [\bar{S}_\theta \rightarrow L^\infty(a, b)]^{|\mathcal{I}|}, \quad s_h \in W^{1,4}(S_\theta), \quad (19)$$

$$\begin{aligned} & s_h \sum_{i \in \mathcal{I}_1} (u_{ih,t}(t), \varphi_i) + (L - s_h) \sum_{i \in \mathcal{I}_2} (u_{ih,t}(t), \varphi_i) + A(s_h, u_h, \varphi) + E(s'_h, u_h + \lambda, \varphi) \\ &= B_F(u_h + \lambda, s_h, \varphi) + H(s'_h, u_h, \varphi) - s_h \sum_{i \in \mathcal{I}} (u_{ih,t}(t), \varphi_i), \end{aligned}$$

$$u'_{4h}(t) = \eta_\Gamma^h(u_h(s_h(t), t), \quad (20)$$

$$s'_h(t) = \eta_\Gamma^h(1, t), \quad (21)$$

for all $\varphi \in \mathbb{V}_h$ a.e. $t \in S_\theta$ and

$$u_h(0) = u_{0h} \in \mathbb{H}, s_h(0) = s_0 > 0. \quad (22)$$

Assumption H: (H1) $\lambda \in W_+^{1,2}(S_T)$, $u_{3,eq} \in L_+^\infty(S_T)$, $u_0 \in L_+^\infty(0, 1)^{|\mathcal{I}_1|} \times L_+^\infty(1, 2)^{|\mathcal{I}_2|}$, $u_{40} \in L_+^\infty(0, s(t))$ a.e. $t \in S_T$; (H2) All coefficients D_i ($i \in \mathcal{I}_1 \cup \mathcal{I}_2$), P_1, P_2, Q_1, Q_2 , and $S_{3,diss}$ are strictly positive; (H3) Assumptions (A)–(C) listed in [7], which ensure the existence of L^∞ -bounds on u and s' , hold here too.

Let (u, s) and (u_h, s_h) be weak solutions to P_Γ and P_Γ^{sd} , i.e. (u, s) and (u_h, s_h) are in agreement with Definition 3.1 and Definition 3.2. Our main result is the following.

Theorem 3.3. Let $u_0 \in \prod_{i \in \mathcal{I}_1 \cup \mathcal{I}_2} V_i \times H^2(a, b)$ and consider assumption (H) be satisfied.

(i) Then the problems P_Γ and P_Γ^{sd} are uniquely solvable.

(ii) There exist a $\rho \in S_T$ and strictly positive constants c_k ($k = 1, 2, 3$), which are independent on h , such that the following estimates hold:

$$\|u - u_h\|_{L^2(S_\rho, \mathbb{V})} \leq c_1 (h^2 + |s - s_h|_{W^{1,4}(S_\rho)}), \quad (23)$$

$$|s' - s'_h|_{L^2(S_\rho)} \leq c_2 h, \quad (24)$$

$$\|u - u_h\|_{L^\infty(S_\rho, \mathbb{H}) \cap L^2(S_\rho, \mathbb{V})} + \|s - s_h\|_{W^{1,4}(S_\rho)} \leq c_3 h. \quad (25)$$

Remark 1. It is worth noting that Theorem 3.3 recovers known results² from the one-phase case stated Theorem 5.1 in [9]. Moreover, we observe that u_4 satisfies the estimate (24) as well.

4. Proof of Theorem 3.3. The proof of (i) relies on the use of fixed-point principles as in [7, 9] or [10]. In this section, we only sketch the proof of (ii). Testing by $w_h \in \mathbb{V}_h$ in both the weak formulation and its semi-discrete counterpart and then subtracting the results, we obtain

$$\begin{aligned} & \sum_{i \in \mathcal{I} - \{4, 5, 6\}} ((u_i + \lambda_i)_t, w_{ih}) - ((u_{ih} + \lambda_i)_t, w_{ih}) + \frac{1}{s^2} \sum_{i \in \mathcal{I}_1 - \{5\}} (D_i u_{i,y}, w_{ih,y}) - \\ & - \frac{1}{s_h^2} \sum_{i \in \mathcal{I}_1 - \{5\}} (D_i u_{ih,y}, w_{ih,y}) + \frac{1}{(L-s)^2} \sum_{i \in \mathcal{I}_2 - \{6\}} (D_i u_{i,y}, w_{ih,y}) \\ & - \frac{1}{(L-s_h)^2} \sum_{i \in \mathcal{I}_2 - \{6\}} (D_i u_{ih,y}, w_{ih,y}) = -\frac{\eta_\Gamma(1)}{s} w_1(1) + \frac{\eta_\Gamma^h(1)}{s_h} w_{1h}(1) \\ & + \sum_{\ell=1}^2 \frac{s'}{s} (u_\ell(1) + \lambda_\ell) w_\ell(1) - \sum_{\ell=1}^2 \frac{s'_h}{s_h} (u_{1h}(1) + \lambda_1) w_{1h}(1) \\ & - \frac{\eta_\Gamma(1)}{L-s} w_3(1) + \frac{\eta_\Gamma^h(1)}{L-s_h} w_{3h}(1) \\ & + \frac{s'}{L-s} (u_3(1) + \lambda_3) w_3(1) - \frac{s'_h}{L-s_h} (u_{3h}(1) + \lambda_3) w_{3h}(1) - P_1(u_1 - Q_1 u_2, w_1) \\ & + P_1(u_{1h} - Q_1 u_{2h}, w_{1h}) + P_2(u_1 - Q_2 u_2, w_2) - P_2(u_{1h} - Q_2 u_{2h}, w_{2h}) \\ & - S_{3,diss}(u_3 - u_{3,eq}, w_{3h}) + S_{3,diss}(u_{3h} - u_{3,eq}, w_{3h}) + \sum_{\ell=1}^2 \frac{s'}{s} (y u_{\ell,y}, w_\ell) \\ & - \sum_{\ell=1}^2 \frac{s'_h}{s_h} (y u_{\ell h,y}, w_\ell) + \frac{s'}{L-s} ((2-y) u_{3,y}, w_{3h}) - \frac{s'_h}{L-s_h} ((2-y) u_{3h,y}, w_{3h}) \quad (26) \end{aligned}$$

and

$$\begin{aligned} & \sum_{j=5}^6 ((u_j + \lambda_j)_t, s w_{jh}) - ((u_{jh} + \lambda_j)_t, s_h w_{jh}) + \frac{D_5}{s} (u_{5,y}, w_{5h,y}) \\ & - \frac{D_5}{s_h} (u_{5h,y}, w_{5h,y}) + \frac{D_6}{L-s} (u_{6,y}, w_{6h,y}) - \frac{D_6}{L-s_h} (u_{6h,y}, w_{6h,y}) \\ & = \eta_\Gamma(1) w_5(1) - \eta_\Gamma^h(1) w_{5h}(1) + s' ((2-y) u_{6,y}, w_{6h}) - s'_h ((2-y) u_{6h,y}, w_{6h}). \quad (27) \end{aligned}$$

In what follows, we deal only with (27) and refer the reader to [9] for a way of estimating (26). We denote $e := u - u_h$, and correspondingly, $e_i := u_i - u_{ih}$ for all

²Of course, the size of the constants c_k and the way they depend on the model parameters is different here than in the one-phase scenario.

$i \in \mathcal{I}$. Grouping conveniently the terms and then dividing the final result by s , we get the following expression:

$$\begin{aligned}
& (e_{5,t}, w_{5h}) + \frac{L-s}{s}(e_{6,t}, w_{6h}) + \frac{D_5}{s^2}(e_{5y}, w_{5h,y}) + \frac{D_6}{(L-s)^2} \frac{L-s}{s}(e_{6,y}, w_{6,y}) \\
&= \frac{s_h-s}{s}(u_{5h,t}, w_{5h}) + \frac{s-s_h}{s}(u_{6h,t}, w_{6h}) + \frac{1}{s} \left(\frac{1}{s} - \frac{1}{s_h} \right) (D_5 u_{5h,y}, w_{5h,y}) \\
&\quad + \frac{1}{s} \left(\frac{1}{L-s_h} - \frac{1}{L-s} \right) (D_6 u_{6h,y}, w_{6h,y}) + \frac{s'-s'_h}{s} w_{5h}(1) \\
&\quad + \frac{s'}{L-s} ((2-y)e_{6,y}, w_{6h}) + \frac{s'_h-s'}{L-s} ((2-y)u_{6h,y}, w_{6h}) \\
&\quad + \frac{s'}{s}(ye_{5,y}, w_{5h}) + \frac{s'_h-s'}{s}(yu_{5h,y}, w_{5h}). \quad (28)
\end{aligned}$$

We denote

$$\hat{d} := (\hat{d}(s(t)) :=) \min_{t \in \bar{S}_T} \left\{ \frac{L-s(t)}{s(t)} \right\} D_6. \quad (29)$$

Note that for all $r \in [s_0, L[$ we have $0 < \hat{d}(r) < \infty$ and $\lim_{r \rightarrow L^-} \frac{\hat{d}(r)}{(L-r)^2} = +\infty$. For convenience of notation, we will not point out anymore the dependence of \hat{d} on $s(t)$. Furthermore, for all $v_h \in \mathbb{V}_h$ we take $w_h = (v_h - u) + e$. Choosing in (28) as test function $w_h = v_h - u_h \in \mathbb{V}_h$, we obtain:

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} (|e_5|^2 + |e_6|^2) + \frac{D_5}{s^2} \|e_5\|^2 + \frac{\hat{d}}{(L-s)^2} \|e_6\|^2 \\
& \leq (e_{5,t}, u_5 - u_{5h}) + (e_{6,t}, u_6 - u_{6h}) + \frac{D_5}{s^2} (e_{5,y}, (u_5 - u_{5h})_y) \\
& \quad + \frac{\hat{d}}{(L-s)^2} (e_{6,y}, (u_6 - u_{6h})_y) = \sum_{\ell=5}^6 (e_{\ell,t}, u_\ell - v_{\ell h}) + \frac{D_5}{s^2} (e_{5,y}, (u_5 - v_{5h})_y) \\
& \quad + \frac{\hat{d}}{(L-s)^2} (e_{6,y}, (u_6 - v_{6h})_y) + \sum_{\ell=5}^6 (e_{\ell,t}, v_{\ell h} - u_{\ell h}) + \frac{D_5}{s^2} (e_{5,y}, (v_{5h} - u_{5h})_y) \\
& \quad + \frac{\hat{d}}{(L-s)^2} (e_{6,y}, (v_{6h} - u_{6h})_y). \quad (30)
\end{aligned}$$

Remark 2. (1) We need to estimate the non-standard terms $(yu_{ih,y}, v_{ih} - u_{ih})$ for all $i \in \mathcal{I}_1$ and $((2-y)u_{ih,y}, v_{ih} - u_{ih})$ for all $i \in \mathcal{I}_2$. We illustrate here our strategy when $i \in \mathcal{I}_1$. Integrating by parts in $\int_0^1 yu_{ih,y}(v_{ih} - u_{ih})dy$ and employing the L^∞ -bounds on (semi-discrete) concentrations, the interpolation inequality as well as the Cauchy-Schwarz's inequality, we obtain

$$\begin{aligned}
| (yu_{ih,y}, v_{ih} - u_{ih}) | & \leq u_{ih}(1) |v_{ih}(1) - u_{ih}(1)| + |u_{ih}| |v_{ih} - u_{ih}| + |u_{ih}| |v_{ih} - u_{ih}| \\
& \leq |u_{ih}(1)| \hat{c} |v_{ih} - u_{ih}|^\theta |v_{ih} - u_{ih}|^{1-\theta} + |u_{ih}| (|v_{ih} - u_{ih}| + |v_{ih} - u_{ih}|) \\
& \leq \bar{c} (|v_{ih} - u_{ih}| + |v_{ih} - u_{ih}|), \quad (31)
\end{aligned}$$

where $\bar{c} := k_1 \left(\hat{c}^{\frac{2}{1-\theta}} + 1 \right)$.

(2) Let \mathcal{R}_h be the Riesz's projection operator. Its properties needed here can be summarized as follows: For any $f \in H^2(a, b)$, there exist the strictly positive constants γ_k ($k = 1, 2, 3$), which are independent of the mesh size h , such that the Lagrange interpolant $\mathcal{R}_h f$ satisfies the inequalities $|f - \mathcal{R}_h f| \leq \gamma_1 h^2 |f|_{H^2(a,b)}$,

$\|f - \mathcal{R}_h f\| \leq \gamma_2 h \|f\|_{H^2(a,b)}$, and $|f(1) - \mathcal{R}_h f(1)| \leq \gamma_3 h^{2-\theta} \|f\|_{H^2(a,b)}$. For details, see Lemma 3.2 in [9] and Theorem 5.5, p. 65 in [4].

Combining (28), (30), and the estimates mentioned in Remark 2, we obtain

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} (|e_5|^2 + |e_6|^2) + \frac{D_5}{s^2} \|e_5\|^2 + \frac{\hat{d}}{(L-s)^2} \|e_6\|^2 \\
& \leq \frac{s_h - s}{s} |u_{5h,t}| |v_{5h} - u_{5h}| + \frac{s_h - s}{s} |u_{6h,t}| |v_{6h} - u_{6h}| \\
& + \sum_{\ell=5}^6 |e_{\ell,t}| |u_\ell - v_{\ell h}| + \frac{D_5}{s^2} \|e_5\| \|u_5 - v_{5h}\| + \frac{\hat{d}}{(L-s)^2} \|e_6\| \|u_6 - v_{6h}\| \\
& + \frac{|s - s_h|}{s^2 s_h} |D_5 u_{5h,y}| |(v_{5h} - u_{5h})_{,y}| + \frac{|s - s_h|}{s(L-s)(L-s_h)} |D_6 u_{6h,y}| |(v_{6h} - u_{6h})_{,y}| \\
& \quad + |s' - s'_h| \frac{1}{s} |v_{5h}(1) - u_{6h}(1)| \\
& + \frac{s'}{s} \left(\frac{1}{2} |e_6(1)|^2 + \frac{1}{2} |e_6|^2 + \|e_6\| \|v_{6h} - u_{6h}\| \right) + \frac{|s' - s'_h|}{s} |u_{6h,y}| |v_{6h} - u_{6h}| \\
& \quad + \frac{s'}{s} \left(\frac{1}{2} |e_5(1)|^2 + \|e_5\| \|v_{5h} - u_{5h}\| \right) + \frac{s'_h - s'}{s} |u_{5h,y}| |v_{5h} - u_{5h}| \\
& \leq \sum_{\ell=5}^6 |e_{\ell,t}| |u_\ell - v_{\ell h}| + \frac{D_5}{s^2} \|e_5\|^2 \|u_5 - v_{5h}\| + \frac{\hat{d}}{(L-s)^2} \|e_6\| \|u_6 - v_{6h}\| \\
& \quad + \frac{|s_h - s|}{s} |u_{5h,t}| (|v_{5h} - u_5| + |e_5|) + \frac{|s_h - s|}{s} |u_{6h,t}| (|v_{6h} - u_6| + |e_6|) \\
& \quad \quad + \frac{|s - s_h|}{s^2 s_h} |D_5 u_{5h,y}| (|v_{5h} - u_{5h}| + \|e_5\|) \\
& \quad \quad + \frac{|s - s_h|}{s(L-s)(L-s_h)} |D_6 u_{6h,y}| (|v_{6h} - u_{6h}| + \|e_6\|) \\
& \quad + \sum_{\ell=5}^6 |s' - s'_h| \frac{1}{s} (|v_{\ell h}(1) - u_\ell(1)| + |e_\ell(1)| + |e_\ell| + |v_{\ell h} - u_\ell|). \quad (32)
\end{aligned}$$

Finally, we get

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} (|e_5|^2 + |e_6|^2) + \frac{D_5}{s^2} \|e_5\|^2 + \frac{\hat{d}}{(L-s)^2} \|e_6\|^2 \\
& \leq \sum_{\ell=5}^6 |e_{\ell,t}| \gamma_1 h^2 (|u_5|_{H^2(0,1)} + |u_6|_{H^2(1,2)}) + \epsilon \frac{D_5}{s^2} \|e_5\|^2 + c_\epsilon \frac{D_5}{s^2} \gamma_2 h^2 \|u_5\|_{H^2(0,1)} \\
& \quad + \epsilon \frac{\hat{d}}{(L-s)^2} \|e_6\|^2 + c_\epsilon \frac{D_6}{(L-s)^2} \gamma_2 h^2 \|u_6\|_{H^2(1,2)} \\
& \quad \quad + \frac{|s_h - s|}{s} |u_{5h,t}| (\gamma_1 h^2 \|u_5\|_{H^2(0,1)} + |e_5|)
\end{aligned}$$

$$\begin{aligned}
& + \frac{|s_h - s|}{s} |u_{6h,t}| (\gamma_1 h^2 \|u_6\|_{H^2(1,2)} + |e_6|) \\
& + \frac{|s - s_h| D_5 |u_{5h,y}|}{s s_h} (\gamma_2 h \|u_5\|_{H^2(0,1)} + |e_5|) \\
& + \frac{|s - s_h| D_6 |u_{6h,y}|}{s(L-s)(L-s_h)} (\gamma_2 h \|u_6\|_{H^2(1,2)} + |e_6|) \\
& + \sum_{\ell=5}^6 |s' - s'_h| \frac{1}{s} (\gamma_3 h^{2-\theta} \|u_\ell\|_{H^2} + \hat{c} |e_\ell|^\theta |e_\ell|^{1-\theta} + |e_\ell| + \gamma_1 h^2 \|u_\ell\|_{H^2}) = \sum_{j=1}^7 I_j, \quad (33)
\end{aligned}$$

where the terms I_j ($j \in \{1, \dots, 7\}$) are defined as follows:

$$\begin{aligned}
I_1 & := \sum_{\ell=5}^6 |e_{\ell,t}| \gamma_1 h^2 (\|u_5\|_{H^2(0,1)} + \|u_6\|_{H^2(1,2)}) \\
I_2 & := \epsilon \frac{D_5}{s^2} \|e_5\|^2 + c_\epsilon \frac{D_5}{s^2} \gamma_2 h^2 \|u_5\|_{H^2(0,1)} \\
& \quad + \epsilon \frac{\hat{d}}{(L-s)^2} \|e_6\|^2 + c_\epsilon \frac{D_6}{(L-s)^2} \gamma_2 h^2 \|u_6\|_{H^2(1,2)} \\
I_3 & := \frac{|s_h - s|}{s} |u_{5h,t}| (\gamma_1 h^2 \|u_5\|_{H^2(0,1)} + |e_5|) \\
I_4 & := \frac{|s_h - s|}{s} |u_{6h,t}| (\gamma_1 h^2 \|u_6\|_{H^2(1,2)} + |e_6|) \\
I_5 & := \frac{|s - s_h| D_5 |u_{5h,y}|}{s s_h} (\gamma_2 h \|u_5\|_{H^2(0,1)} + |e_5|) \\
I_6 & := \frac{|s - s_h| D_6 |u_{6h,y}|}{s(L-s)(L-s_h)} (\gamma_2 h \|u_6\|_{H^2(1,2)} + |e_6|) \\
I_7 & := \sum_{\ell=5}^6 |s' - s'_h| \frac{1}{s} (\gamma_3 h^{2-\theta} \|u_\ell\|_{H^2} + \hat{c} |e_\ell|^\theta |e_\ell|^{1-\theta} + |e_\ell| + \gamma_1 h^2 \|u_\ell\|_{H^2}).
\end{aligned}$$

By $e_{\ell,t} \in L^2(S_\rho, L^2(a, b))$ ($\ell = 5, 6$) for $\rho \in]0, \min\{\theta, \delta\}$ and the standard energy estimates for the continuous problem [7], we note that all I_j are bounded from above. After manipulating elementary inequalities, we obtain:

$$\begin{aligned}
I_1 & \leq \sum_{\ell=5}^6 \frac{|e_{\ell,t}|^2}{2} h^2 + \frac{\gamma_1 h^2}{2} (\|u_5\|_{H^2(0,1)}^2 + \|u_6\|_{H^2(1,2)}^2) \\
I_2 & \leq \epsilon \frac{D_5}{s^2} \|e_5\|^2 + \epsilon \frac{\hat{d}}{(L-s)^2} \|e_6\|^2 + c_\epsilon \gamma_2^2 \left(\frac{D_5}{s^2} + \frac{D_6}{(L-s)^2} \right) (\|u_5\|_{H^2}^2 + \|u_6\|_{H^2}^2) \\
I_3 & \leq |s_h - s|^2 + \frac{\gamma_1}{2} |u_{5h,t}|^2 \|u_5\|_{H^2}^2 h^4 + \frac{\gamma_1^2}{2} |u_{5h,t}|^2 |e_5|^2 \\
I_4 & \leq |s_h - s|^2 + \frac{\gamma_1}{2} |u_{6h,t}|^2 \|u_6\|_{H^2}^2 h^4 + \frac{\gamma_1^2}{2} |u_{6h,t}|^2 |e_6|^2
\end{aligned}$$

$$\begin{aligned}
I_5 &\leq \frac{1}{2} \left(1 + \frac{c_\epsilon D_5^2 |u_{5h,y}|^2}{2s_h^2} \right) |s - s_h^2| + \frac{\gamma_2^2 D_5 |u_{5h,y}|^2}{2s^2 s_h^2} \|u_5\|_{H^2}^2 h^2 \\
&\quad + c_\epsilon \frac{|s - s_h|^2 D_5^2 |u_{5h,y}|^2}{2s_h^2} + \epsilon \frac{\|e_5\|^2}{s^2} \\
I_6 &\leq \frac{1}{2} \left(1 + \frac{c_\epsilon D_6^2 |u_{6h,y}|^2}{2s^2 (L - s_h)^2} \right) |s - s_h^2| + \frac{\gamma_2^2 D_6 |u_{6h,y}|^2}{2s^2 (L - s)^2 (L - s_h)^2} \|u_6\|_{H^2}^2 h^2 \\
&\quad + \epsilon \frac{\|e_6\|^2}{(L - s)^2} \\
I_7 &\leq \sum_{\ell=5}^6 \left[\frac{|s' - s'_h|^2}{2} + \frac{\gamma_3^2}{s^2} h^{2(2-\theta)} |u_\ell|_{H^2}^2 \right] + \bar{\zeta} |s' - s'_h|^2 + \zeta c_{\bar{\zeta}} \frac{\|e_5\|^2}{s^2} \\
&\quad + \zeta c_{\bar{\zeta}} \frac{\|e_6\|^2}{(L - s)^2} + c_\epsilon c_{\bar{\zeta}} (\gamma_3 \hat{c})^{\frac{2}{1-\theta}} \left(\frac{L - s}{s} \right)^{\frac{2}{1-\theta}} |e_6|^2 + c_\zeta c_{\bar{\zeta}} (\gamma_3 \hat{c})^{\frac{2}{1-\theta}} |e_5|^2 \\
&\quad + \sum_{\ell=5}^6 \frac{|e_\ell|^2}{2} + \frac{3}{2} |s - s'_h|^2 + \frac{\gamma_1^2}{2} \sum_{\ell=5}^6 |u_\ell|_{H^2}^2 h^4.
\end{aligned}$$

Finally, we estimate $\sum_{j=1}^7 I_j$ by

$$\begin{aligned}
\sum_{j=1}^7 I_j &\leq |s - s_h|^2 \left(3 + c_\zeta \frac{D_5^2 |u_{5h,y}|^2}{2s_h^2} + \frac{c_\zeta D_6^2 |u_{6h,y}|^2}{2s^2 (L - s_h)^2} \right) + |s' - s'_h| \left(\frac{7}{2} + \bar{\zeta} \right) \\
&\quad + \frac{\|e_5\|^2}{s^2} (\epsilon D_5 + \zeta c_{\bar{\zeta}}) + \frac{\|e_6\|^2}{(L - s)^2} (\epsilon \hat{d} + \zeta c_{\bar{\zeta}}) \\
&\quad + h^2 \left(\sum_{\ell=5}^6 |e_{\ell,t}|^2 + \frac{\gamma_1}{2} (\|u_5\|_{H^2} + \|u_6\|_{H^2}) + \frac{\gamma_1^2}{2} |u_{5h,t}|^2 |u_5|_{H^2}^2 + \frac{\gamma_1^2}{2} |u_{6h,t}|^2 |u_6|_{H^2}^2 + \right. \\
&\quad \quad + \frac{\gamma_2^2}{2s^2 s_h^2} D_5^2 |u_{5h,y}|^2 |u_5|_{H^2}^2 + \frac{\gamma_2^2}{2s^2 (L - s)^2 (L - s_h)^2} D_6^2 |u_{6h,y}|^2 |u_6|_{H^2}^2 + \\
&\quad \quad \left. + \frac{\gamma_3^2}{s^2} (\|u_5\|_{H^2}^2 + \|u_6\|_{H^2}^2) + \frac{\gamma_1}{2} (\|u_5\|_{H^2}^2 + \|u_6\|_{H^2}^2) \right) \\
&\quad + (|e_5|^2 + |e_6|^2) \left[\frac{\gamma_1^2}{2} (|u_{5h,t}|^2 + |u_{6h,t}|^2) + c_\zeta c_{\bar{\zeta}} (\gamma_3 \hat{c})^{\frac{2}{1-\theta}} \left(\left(\frac{L}{s} - 1 \right)^{\frac{2}{1-\theta}} + 1 \right) + \frac{1}{2} \right]. \quad (34)
\end{aligned}$$

Note that the second term from the r.h.s. of (34) can be estimated with the help of

$$|s' - s'_h| \leq \|e\|, \quad (35)$$

while the third and the fourth terms can be compensated employing the two 'diffusive' terms from the l.h.s. of (34). We denote $\tilde{D}_5 := D_5 - \epsilon D_5 - \zeta c_{\bar{\zeta}}$ and $\tilde{d} := \hat{d} - \epsilon \hat{d} - \zeta c_{\bar{\zeta}}$ and choose $\epsilon > 0$ and $\zeta c_{\bar{\zeta}} > 0$, such that $\tilde{D}_5 \geq 0$ and $\tilde{d} \geq 0$. Furthermore, using (35), it yields

$$\begin{aligned}
&\frac{d}{dt} (|e_5|^2 + |e_6|^2) + \frac{\tilde{D}_5}{s^2} \|e_5\|^2 + \frac{\tilde{d}}{(L - s)^2} \|e_6\|^2 \\
&\leq \alpha_1(t) h^2 + \alpha_2(t) (|e_5|^2 + |e_6|^2) + \alpha_3(t) |s - s_h|^2. \quad (36)
\end{aligned}$$

In (36), we have $\alpha_i \in L^1_+(S_T)$ ($i \in \{1, 2, 3\}$), while their exact definitions can be read off from (34). It is important to notice that (36) has a nice structure for which Gronwall's inequality can be applied (after adding further terms arising from (26)).

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