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Document status and date:
Published: 01/01/2011

Document Version:
Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
• The final author version and the galley proof are versions of the publication after peer review.
• The final published version features the final layout of the paper including the volume, issue and page numbers.
Link to publication

EINDHOVEN UNIVERSITY OF TECHNOLOGY
Department of Mathematics and Computer Science

Semi-discrete finite difference multiscale scheme for a concrete corrosion model:
approximation estimates and convergence

by

V. Chalupecký, A. Muntean

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Vladimír Chalupecký[*]   Adrian Muntean[†]

June 24, 2011

Abstract

We propose a semi-discrete finite difference multiscale scheme for a concrete corrosion model consisting of a system of two-scale reaction-diffusion equations coupled with an ode. We prove energy and regularity estimates and use them to get the necessary compactness of the approximation estimates. Finally, we illustrate numerically the behavior of the two-scale finite difference approximation of the weak solution.

Keywords Multiscale reaction-diffusion equations · Two-scale finite difference method · Approximation of weak solutions · Convergence · Concrete corrosion

Mathematics Subject Classification (2000) MSC 35K51 · 35K57 · 65M06 · 65M12 · 65M20

1   Introduction

Biogenic sulfide corrosion of concrete is a bacterially mediated process of forming hydrogen sulfide gas and the subsequent conversion to sulfuric acid that attacks concrete and steel within wastewater environments. The hydrogen sulfide gas is oxidized in the presence of moisture to form sulfuric acid that attacks the matrix of concrete. The effect of sulfuric acid on concrete and steel surfaces exposed to severe wastewater environments (like sewer pipes) is devastating, and is always associated with high maintenance costs.

The process can be briefly described as follows: Fresh domestic sewage entering a wastewater collection system contains large amounts of sulfates that, in the absence of dissolved oxygen and nitrates, are reduced by bacteria. Such bacteria identified primarily from the anaerobic species Desulfovibrio lead to the fast formation of hydrogen sulfide (H_2S) via a complex pathway of biochemical reactions. Once the gaseous H_2S diffuses into the headspace environment above the wastewater, a sulfur oxidizing bacteria – primarily Thiobacillus aerobic bacteria – metabolizes the H_2S gas and oxidize it to sulphuric acid. It is worth noting that Thiobacillus colonizes on pipe crowns above the waterline inside the sewage system. This oxidizing process prefers to take place where there is sufficiently high local temperature, enough productions of hydrogen sulfide gas, high relative humidity, and atmospheric oxygen; see section 2.2 for

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[*]Institute of Mathematics for Industry, Kyushu University, 744 Motooka, Nishi-ku, 819-0395 Fukuoka, Japan.
E-mail: chalupecky@imi.kyushu-u.ac.jp

[†]Faculty of Mathematics and Computer Science, CASA - Center for Analysis, Scientific computing and Applications, Institute for Complex Molecular Systems (ICMS), Technical University of Eindhoven, PO Box 513, 5600 MB, Eindhoven, The Netherlands. E-mail: a.muntean@tue.nl

more details on the involved chemistry and transport mechanisms. Good overviews of the civil engineering literature on the chemical aggression with acids of cement-based materials [focussing on sulfate ingress] can be found in [3, 12, 17, 22].

If we decouple the mechanical corrosion part (leading to cracking and respective spalling of the concrete matrix) from the reaction-diffusion-flow part, and look only to the later one, the mathematical problem reduces to solving a partly dissipative reaction-diffusion system posed in heterogeneous domains. Now, assuming further that the concrete sample is perfectly covered by a locally-periodic repeated regular microstructure, averaged and two-scale reaction-diffusion systems modeling this corrosion processes can be derived; that is precisely what we have done in [9] (formal asymptotics for the locally-periodic case) and [21] (rigorous asymptotics via two-scale convergence for the periodic case).

Here, our attention focusses on the two-scale corrosion model. Besides performing the averaging procedure and ensuring the well-posedness of the resulting model(s), we are interested in simulating numerically the influence of the microstructural effects on observable (macroscopic) quantities. We refer the reader to [5], where we performed numerical simulations of such a two-scale model. Now, is the right moment to raise the main question of this paper:

Is the two-scale finite difference scheme used in [5] convergent, i.e., does it approximate the weak solution to the two-scale system?

It is worth mentioning that there is a wealth of multiscale numerical techniques that could (in principle) be used to tackle RD systems of the type treated here. We mention at this point three approaches only: (i) the multiscale FEM method developed by Babuska and predecessors (see the book [8] for more Refs.), (ii) computations on two-scale FEM spaces [16] / two-scale Galerkin approximations [19, 18], and (iii) the philosophy of heterogeneous multiscale methods (HMM) [7]. We choose to employ here multiscale finite differences (multiscale FD) mimicking the [two-scale] tensorial structure present in (ii). Our hope is to become able to marry at a later stage the two-scale Galerkin approximation ideas from [19, 15] in a HMM framework eventually based on finite differences. Our standard reference for FD-HMM idea is [1].

The paper is structured as follows: Section 2 introduces the reader to the physico-chemical background of the corrosion process, two-scale geometry, and setting of the equations. The numerical scheme together with basic ingredients like discrete operators, discrete Green formulae, discrete trace inequalities etc. are presented in section 3, while the approximation estimates together with the interpolation (extension) and compactness steps are the subject of Section 5 . We conclude the paper with Section 6 containing numerical illustrations of the discrete approximation of the weak solution.

2   Background and statement of the problem

2.1   Two-scale geometry

We consider the evolution of a chemical corrosion process (sulfate attack) taking place in one-dimensional macroscopic region $\Omega := (0, L)$, $L > 0$, that represents a concrete sample along a line perpendicular to the pipe surface with $x = 0$ being a point at the inner surface in contact with sewer atmosphere and $x = L$ being a point inside the concrete wall. Since we do not take into account bulging of the inner surface due to the growth of soft gypsum structures, the shape of the domain Ω does not change w.r.t. the time variable t.

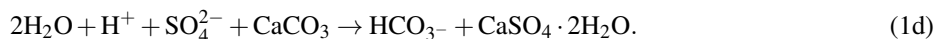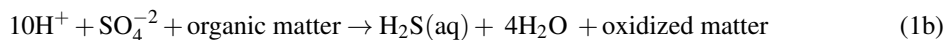We denote the typical microstructure (or standard cell [11]) by $Y := (0, \ell)$, $\ell > 0$. Usually cells in concrete contain a stationary water film, and air and solid fractions in different ratios depending on the local porosity. Generally, we expect that, due to the randomness of the pores distribution in concrete, the choice of the microstructure essentially depends on the macroscopic position $x \in \Omega$, i.e., we would

then have Y_x; see [20] for averaging issues of double porosity media involving locally periodic ways of distributing microstructures, and [9] for more comments directly related to the sulfatation problem where pores are distributed in a locally periodic fashion. In this paper, we restrict to the case when the medium Ω is made of the *same* microstructure Y periodically repeated to pave perfectly the region. Furthermore, since at the microscopic level the involved reaction and diffusion processes take place in the pore water, we choose to denote by Y only the wet part of the pore. Efficient direct computations (with controlled accuracy and known convergence rates) of scenarios involving Y_x as well as the corresponding error analysis are generally open problems in the field of multiscale numerical simulation.

2.2 Chemistry

Sewage is rich in sulphur-containing materials and normally it is without any action on concrete. Under suitable conditions like increased temperature or lower flow velocity oxygen in sewage can become depleted. Aerobic, purifying bacteria become inactive while anaerobic bacteria that live in slime layers at the bottom of the sewer pipe proliferate. They obtain needed oxygen by reducing sulfur compounds. Sulfur reacts with hydrogen and forms hydrogen sulfide (H_2S), which then diffuses in sewage and enters sewer atmosphere. It moves in the air space of the pipe and goes up towards the pipe wall. Gaseous H_2S (further denoted as $H_2S(g)$) enters into the concrete pores (microstructures) via both air and water parts. $H_2S(g)$ diffuses quickly through the air-filled part of the porous structure over macroscopic distances, while it dissolves in the thin, stationary water film of much smaller, microscopic thickness that clings on the surface of the fabric.

There are many chemical reactions taking place in the porous microstructure of sewer pipes which degrade the performance of the pipe structure depending on the intensity of the interaction between the chemical reactions and the local environment. Here we focus our attention on the following few relevant chemical reactions:

$$H_2S(aq) + 2O_2 \rightarrow 2H^+ + SO_4^{2-} \tag{1a}$$

$$10H^+ + SO_4^{-2} + \text{organic matter} \rightarrow H_2S(aq) + 4H_2O + \text{oxidized matter} \tag{1b}$$

$$H_2S(aq) \rightleftharpoons H_2S(g) \tag{1c}$$

$$2H_2O + H^+ + SO_4^{2-} + CaCO_3 \rightarrow HCO_{3-} + CaSO_4 \cdot 2H_2O. \tag{1d}$$

Dissolved hydrogen sulfide (further denoted as $H_2S(aq)$) undergoes oxidation by aerobic bacteria living in these films and sulfuric acid H_2SO_4 is produced (reaction (1a)). This aggressive acid reacts with calcium carbonate (i.e., with our concrete sample) and a soft gypsum layer ($CaSO_4 \cdot 2H_2O$) consisting of solid particles (unreacted cement, aggregate), pore air and moisture is formed (reaction (1d)).

The model considered in this paper pays special attention to the following aspects:

(i) exchange of H_2S from water to the air phase and vice versa (reaction (1c);

(ii) production of gypsum at micro solid-water interfaces (reaction (1d)).

The transfer of H_2S is modeled by means of (deviations from) the Henry's law, while the production of gypsum is incorporated in a non-standard non-linear reaction rate, here denoted as η; see (6) for a precise choice. Equation (7) indicates the linearity of the Henry's law structure we have in mind. The standard reference for modeling gas-liquid reactions at stationary interfaces (including a derivation via first principles of the Henry's law) is [6].

2.3 Setting of the equations

Let $S := (0, T)$ (with $T \in (0, \infty)$) be the time interval during which we consider the process and let Ω and Y as described in section 2.1. We look for the unknown functions (mass concentrations of active chemical

species)

$$u_1 : \Omega \times S \to \mathbb{R} \qquad\qquad\qquad\qquad \text{– concentration of } H_2S(g),$$
$$u_2 : \Omega \times Y \times S \to \mathbb{R} \qquad\qquad\qquad \text{– concentration of } H_2S(aq),$$
$$u_3 : \Omega \times Y \times S \to \mathbb{R} \qquad\qquad\qquad \text{– concentration of } H_2SO_4,$$
$$u_4 : \Omega \times S \to \mathbb{R} \qquad\qquad\qquad\qquad \text{– concentration of gypsum,}$$

that satisfy the following two-scale system composed of three weakly coupled PDEs and one ODE

$$\partial_t u_1 - d_1 \partial_{xx} u_1 = d_2 \partial_y u_2|_{y=0}, \qquad\qquad \text{in } \Omega, \qquad\qquad (2a)$$
$$\partial_t u_2 - d_2 \partial_{yy} u_2 = -\zeta(u_2, u_3), \qquad\qquad \text{in } \Omega \times Y, \qquad\qquad (2b)$$
$$\partial_t u_3 - d_3 \partial_{yy} u_3 = \zeta(u_2, u_3), \qquad\qquad \text{in } \Omega \times Y, \qquad\qquad (2c)$$
$$\partial_t u_4 = \eta(u_3|_{y=\ell}, u_4), \qquad\qquad \text{in } \Omega, \qquad\qquad (2d)$$

together with boundary conditions

$$u_1 = u_1^D, \qquad\qquad\qquad \text{on } \{x=0\} \times S, \qquad\qquad (3a)$$
$$d_1 \partial_x u_1 = 0, \qquad\qquad\qquad \text{on } \{x=L\} \times S, \qquad\qquad (3b)$$
$$-d_2 \partial_y u_2 = Bi^M(H u_1 - u_2), \qquad\qquad \text{on } \Omega \times \{y=0\} \times S, \qquad\qquad (3c)$$
$$d_2 \partial_y u_2 = 0, \qquad\qquad\qquad \text{on } \Omega \times \{y=\ell\} \times S, \qquad\qquad (3d)$$
$$-d_3 \partial_y u_3 = 0, \qquad\qquad\qquad \text{on } \Omega \times \{y=0\} \times S, \qquad\qquad (3e)$$
$$d_3 \partial_y u_3 = -\eta(u_3, u_4), \qquad\qquad \text{on } \Omega \times \{y=\ell\} \times S, \qquad\qquad (3f)$$

and initial conditions

$$
\begin{aligned}
u_1 &= u_1^0, \quad \text{on } \Omega \times \{t=0\}, \\
u_2 &= u_2^0, \quad \text{on } \Omega \times Y \times \{t=0\}, \\
u_3 &= u_3^0, \quad \text{on } \Omega \times Y \times \{t=0\}, \\
u_4 &= u_4^0, \quad \text{on } \Omega \times \{t=0\}.
\end{aligned}
\qquad\qquad (4)
$$

Here d_k, $k \in \{1,2,3\}$, are the diffusion coefficients, Bi^M is a dimensionless Biot number, H is the Henry's constant, α, β are air-water mass transfer functions, while $\eta(\cdot)$ is a surface chemical reaction. Note that u_i ($i = 1, \ldots, 4$) are mass concentrations. Furthermore, all unknown functions, data and parameters carry dimensions.

2.3.1 Technical assumptions

The initial and boundary data, the parameters as well as the involved chemical reaction rate are assumed to satisfy the following requirements:

(A1) $d_k > 0$, $k \in \{1,2,3\}$, $Bi^M > 0$, $H > 0$, $u_1^D > 0$ are constants;

(A2) The function ζ represents the biological oxidation volume reaction between the hydrogen sulfide and sulfuric acid and is defined by

$$\zeta : \mathbb{R}^2 \to \mathbb{R}, \ \zeta(r,s) := \alpha r - \beta s, \qquad\qquad (5)$$

where $\alpha, \beta \in L_+^\infty(Y)$.

(A3) We assume the reaction rate $\eta : \mathbb{R}^2 \to \mathbb{R}_+$ takes the form

$$\eta(r,s) = \begin{cases} kR(r)Q(s), & \text{for all } r \geq 0, s \geq 0, \\ 0, & \text{otherwise,} \end{cases} \qquad\qquad (6)$$

where $k > 0$ is the corresponding reaction constant. We assume η to be (globally) Lipschitz in both arguments. Furthermore, R is taken to be sublinear (i.e., $R(r) \le r$ for all $r \in \mathbb{R}$, in the spirit of [2]), while Q is bounded from above by a threshold $\bar{c} > 0$. Furthermore, let $R \in W^{1,\infty}(0, M_3)$ and $Q \in W^{1,\infty}(0, M_4)$ be monotone functions (with R strictly increasing), where the constants M_3 and M_4 are the L^∞ bounds on u_3 and, respectively, on u_4. Note that [5, Lemma 2] gives the constants M_3, M_4 explicitly.

(A4) $u_1^0 \in H^2(\Omega) \cap L^\infty_+(\Omega)$, $(u_2^0, u_3^0) \in \left[L^2(\Omega; H^1(Y))\right]^2 \times \left[L^\infty_+(\Omega \times Y)\right]^2$, $u_4^0 \in H^1(\Omega) \cap L^\infty_+(\Omega)$;

2.3.2 Micro-macro transmission

Terms like

$$Bi^M \left(H u_1(x,t) - u_2(x, y = 0, t)\right) \tag{7}$$

are usually referred to in the mathematical literature as production terms by Henry's or Raoult's law; see [4]. The special feature of our scenario is that the term (7) *bridges* two distinct spatial scales: one macro with $x \in \Omega$ and one micro with $y \in Y$. We call this *micro-macro transmission condition*.

It is important to note that in the subsequent analysis we can replace (7) by a more general nonlinear relationship

$$\mathcal{B}(u_1, u_2).$$

In that case assumption (A2) needs to be replaced, for instance, by (A2')

$$\mathcal{B} \in C^1\left([0, M_1] \times [0, M_2]; \mathbb{R}\right), \mathcal{B} \text{ globally Lipschitz in both arguments}, \tag{8}$$

where M_1 and M_2 are sufficiently large positive constants[1]. Note that a derivation of the precise structure of $\mathcal{B}$ by taking into account (eventually by averaging of) the underlying microstructure information is still an open problem.

2.4 Weak formulation

As a next step, we first reformulate our problem (2), (3), (4) in an equivalent formulation that is more suitable for numerical treatment. We introduce the substitution $\tilde{u}_1 := u_1 - u_1^D$ to obtain

$$
\begin{aligned}
\partial_t \tilde{u}_1 - d_1 \partial_{xx} \tilde{u}_1 &= d_2 \partial_y u_2|_{y=0}, & \text{in } \Omega, & \tag{9a} \\
\partial_t u_2 - d_2 \partial_{yy} u_2 &= -\zeta(u_2, u_3), & \text{in } \Omega \times Y, & \tag{9b} \\
\partial_t u_3 - d_3 \partial_{yy} u_3 &= \zeta(u_2, u_3), & \text{in } \Omega \times Y, & \tag{9c} \\
\partial_t u_4 &= \eta(u_3|_{y=\ell}, u_4), & \text{in } \Omega, & \tag{9d}
\end{aligned}
$$

together with boundary conditions

$$
\begin{aligned}
\tilde{u}_1 &= 0, & \text{on } \{x = 0\} \times S, & \tag{10a} \\
d_1 \partial_x \tilde{u}_1 &= 0, & \text{on } \{x = L\} \times S, & \tag{10b} \\
-d_2 \partial_y u_2 &= Bi^M \left(H(\tilde{u}_1 + u_1^D) - u_2\right), & \text{on } \Omega \times \{y = 0\} \times S, & \tag{10c} \\
d_2 \partial_y u_2 &= 0, & \text{on } \Omega \times \{y = \ell\} \times S, & \tag{10d} \\
-d_3 \partial_y u_3 &= 0, & \text{on } \Omega \times \{y = 0\} \times S, & \tag{10e} \\
d_3 \partial_y u_3 &= -\eta(u_3, u_4), & \text{on } \Omega \times \{y = \ell\} \times S, & \tag{10f}
\end{aligned}
$$

---

[1] Typical choices for M_1, M_2 are the L^∞-estimates on u_1 and u_2; cf. [5] (Lemma 2) such M_1, M_2 do exist.

and initial conditions

$$
\begin{aligned}
\tilde{u}_1 &= u_1^0 - u_1^D =: \tilde{u}_1^0, &&\text{on } \Omega \times \{t = 0\}, \\
u_2 &= u_2^0, &&\text{on } \Omega \times Y \times \{t = 0\}, \\
u_3 &= u_3^0, &&\text{on } \Omega \times Y \times \{t = 0\}, \\
u_4 &= u_4^0, &&\text{on } \Omega \times \{t = 0\}.
\end{aligned}
\tag{11}
$$

We refer to the system (9), (10), (11) as problem (P). Also, for the ease of notation, we denote $\tilde{u}_1$ again as u_1 and $\tilde{u}_1^0$ as u_1^0.

Now, we can introduce our concept of weak solution.

Definition 1 (Concept of weak solution). The vector of functions (u_1, u_2, u_3, u_4) with

$$
u_1 \in L^2(S, H_0^1(\Omega)), \tag{12}
$$
$$
\partial_t u_1 \in L^2(S \times \Omega), \tag{13}
$$
$$
u_i \in L^2(S, L^2(\Omega, H^1(Y))), \qquad i \in \{2,3\}, \tag{14}
$$
$$
\partial_t u_i \in L^2(S \times \Omega \times Y), \qquad i \in \{2,3\}, \tag{15}
$$
$$
u_4(\cdot, x, y) \in H^1(S), \qquad \text{for a.e. } (x,y) \in \Omega \times Y, \tag{16}
$$

is called *a weak solution* to problem (P) if the identities

$$
\int_\Omega \partial_t u_1 \varphi_1 + d_1 \int_\Omega \partial_x u_1 \partial_x \varphi_1 = \int_\Omega \partial_y u_2|_{y=0} \varphi_1,
$$
$$
\int_\Omega \int_Y \partial_t u_2 \varphi_2 + d_2 \int_\Omega \int_Y \partial_y u_2 \partial_y \varphi_2 = -\int_\Omega \int_Y \zeta(u_2, u_3) \varphi_2 - \int_\Omega \partial_y u_2|_{y=0} \varphi_2,
$$
$$
\int_\Omega \int_Y \partial_t u_3 \varphi_3 + d_3 \int_\Omega \int_Y \partial_y u_3 \partial_y \varphi_3 = \int_\Omega \int_Y \zeta(u_2, u_3) \varphi_3 - \int_\Omega \eta(u_3|_{y=\ell}, u_4) \varphi_3,
$$

and

$$
\partial_t u_4 = \eta(u_3|_{y=\ell}, u_4),
$$

hold for a.e. $t \in S$ and for all $\varphi := (\varphi_1, \varphi_2, \varphi_3) \in H_0^1(\Omega) \times \left[L^2(\Omega; H^1(Y)) \right]^2$.

We refer the reader to [5, Theorem 3] for statements regarding the global existence and uniqueness of such weak solutions to problem (P); see also [19] for the analysis on a closely related problem.

The main question we are dealing with here is:

How to approximate the weak solution in an easy and efficient way, consistent with the structure of the model and the regularity of the data and parameters indicated in (A1)–(A4)?

3 Numerical scheme

In order to solve numerically our multiscale system (2)–(4), we use a semi-discrete approach leaving the time variable continuous and discretizing both space variables x and y by finite differences on rectangular grids. In the following paragraphs we introduce the necessary notation, the scheme and discrete scalar products and norms.

3.1 Grids and grid functions

For spatial discretization, we subdivide the domain Ω into N_x equidistant subintervals, the domain Y into N_y equidistant subintervals and we denote by $h_x := L/N_x$, $h_y := \ell/N_y$, the corresponding spatial step sizes. We denote by h the vector (h_x, h_y) with length $|h|$.

Let

$$
\begin{aligned}
\Omega_h &:= \{x_i := ih_x \mid i = 0, \ldots, N_x\}, \\
\Omega_h^o &:= \{x_i \mid i = 1, \ldots, N_x\}, \\
Y_h &:= \{y_j := jh_y \mid i = 0, \ldots, N_y\}, \\
\Omega_h^e &:= \{x_{i+1/2} := (i+1/2)h_x \mid i = 0, \ldots, N_x - 1\}, \\
Y_h^e &:= \{y_{j+1/2} := (j+1/2)h_y \mid i = 0, \ldots, N_y - 1\},
\end{aligned}
$$

be, respectively, grid of all nodes in Ω, grid of nodes in Ω without the node at $x = 0$ (where Dirichlet boundary condition will be imposed), grid of all nodes in Y, grid of nodes located in the middle of subintervals of Ω_h, and grid of nodes located in the middle of subintervals of Y_h. Finally, we define grids $\omega_h := \Omega_h \times Y_h$ and $\omega_h^e := \Omega_h \times Y_h^e$.

Next, we introduce grid functions defined on the grids just described. Let $\mathcal{G}_h := \{u_h \mid u_h : \Omega_h \to \mathbb{R}\}$, $\mathcal{G}_h^o := \{u_h \mid u_h : \Omega_h^o \to \mathbb{R}\}$ and $\mathcal{E}_h := \{v_h \mid v_h : \Omega_h^e \to \mathbb{R}\}$ be sets of grid functions approximating macro variables on Ω. Let $\mathcal{F}_h := \{u_h \mid u_h : \omega_h \to \mathbb{R}\}$ and $\mathcal{H}_h := \{v_h \mid v_h : \omega_h^e \to \mathbb{R}\}$ be sets of grid functions approximating micro variables on $\Omega \times Y$. These grid functions can be identified with vectors in $\mathbb{R}^N$, whose elements are the values of the grid function at the nodes of the respective grid. Hence, addition of functions and multiplication of a function by a scalar are defined as for vectors.

For $u_h \in \mathcal{G}_h$ we denote $u_i := u_h(x_i)$, and for $u_h \in \mathcal{F}_h$ we will denote $u_{ij} := u_h(x_i, y_j)$. For $v_h \in \mathcal{E}_h$ we will denote $v_{i+1/2} := v_h(x_{i+1/2})$, and for $v_h \in \mathcal{H}_h$ we will denote $v_{i,j+1/2} := v_h(x_i, y_{j+1/2})$.

We frequently use functions from $\mathcal{F}_h$ restricted to the sets $\Omega_h \times \{y = 0\}$ or $\Omega_h \times \{y = \ell\}$. For $u_h \in \mathcal{F}_h$, we will denote these restrictions as $u_h|_{y=0}$ and $u_h|_{y=\ell}$, and we will interpret them as functions from $\mathcal{G}_h$, i.e., $u_h|_{y=0} \in \mathcal{G}_h$ and $u_h|_{y=\ell} \in \mathcal{G}_h$.

3.2 Discrete operators

In this section, we define difference operators defined on linear spaces of grid functions in such a way they mimic properties of the corresponding differential operators and, together with the scalar products defined in Sec. 3.4, fulfill similar integral identities.

The discrete gradient operators ∇_h and ∇_{yh} are defined as

$$
\nabla_h : \mathcal{G}_h \to \mathcal{E}_h, \qquad (\nabla_h u_h)_{i+\frac{1}{2}} := \frac{u_{i+1} - u_i}{h_x}, \quad u_h \in \mathcal{G}_h,
$$

$$
\nabla_{yh} : \mathcal{F}_h \to \mathcal{H}_h, \qquad (\nabla_{yh} u_h)_{i,j+\frac{1}{2}} := \frac{u_{i,j+1} - u_{ij}}{h_y}, \quad u_h \in \mathcal{F}_h,
$$

while the discrete divergence operators div_h and div_{yh} is

$$
\text{div}_h : \mathcal{E}_h \to \mathcal{G}_h^o, \qquad (\text{div}_h v_h)_i := \frac{v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}}{h_x}, \quad v_h \in \mathcal{E}_h,
$$

$$
\text{div}_{yh} : \mathcal{H}_h \to \mathcal{F}_h, \qquad (\text{div}_{yh} v_h)_{ij} := \frac{v_{i,j+\frac{1}{2}} - v_{i,j-\frac{1}{2}}}{h_y}, \quad v_h \in \mathcal{H}_h.
$$

The discrete Laplacian operators Δ_h and Δ_{yh} are defined as $\Delta_h := \mathrm{div}_h \nabla_h : \mathscr{G}_h \to \mathscr{G}_h^o$ and $\Delta_{yh} := \mathrm{div}_{yh} \nabla_{yh} : \mathscr{F}_h \to \mathscr{F}_h$, i.e., the following standard 3-point stencils are obtained:

$$(\Delta_h u_h)_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{h_x^2}, \qquad u_h \in \mathscr{G}_h,$$

$$(\Delta_{yh} u_h)_{ij} = \frac{u_{i,j-1} - 2u_{ij} + u_{i,j+1}}{h_y^2}, \qquad u_h \in \mathscr{F}_h.$$

To complete the definition of the discrete divergence and Laplacian operators, we need to specify values of grid functions on auxiliary nodes that fall outside their corresponding grid. At a later point, we obtain these values from the discretization of boundary conditions by centered differences.

3.3 Semi-discrete scheme

We can now construct a semi-discrete scheme for problem (2). Note that we omit the explicit dependence on t and we interchangeably use the notation $\frac{du_h}{dt}$ and $\dot{u}_h$ for denoting the derivative of u_h with respect to t.

Definition 2. A quadruple $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ with

$$u_h^1, u_h^4 \in C^1([0,T]; \mathscr{G}_h) \text{ and } u_h^2, u_h^3 \in C^1([0,T]; \mathscr{F}_h)$$

is called semi-discrete solution of (2), if it satisfies the following system of ordinary differential equations

$$\frac{du_h^1}{dt} = d_1 \Delta_h u_h^1 - Bi^M \left(H(u_h^1 + u_1^D) - u_h^2|_{y=0} \right), \qquad \text{on } \Omega_h^o, \tag{17a}$$

$$\frac{du_h^2}{dt} = d_2 \Delta_{yh} u_h^2 - \zeta(u_h^2, u_h^3), \qquad \text{on } \omega_h, \tag{17b}$$

$$\frac{du_h^3}{dt} = d_3 \Delta_{yh} u_h^3 + \zeta(u_h^2, u_h^3), \qquad \text{on } \omega_h, \tag{17c}$$

$$\frac{du_h^4}{dt} = \eta(u_h^3|_{y=\ell}, u_h^4), \qquad \text{on } \Omega_h, \tag{17d}$$

together with the discrete boundary conditions ($i = 0, \ldots, N_x$)

$$u_0^1 = 0, \tag{18a}$$

$$d_1 \frac{1}{2} \left((\nabla_h u_h^1)_{N_x + \frac{1}{2}} + (\nabla_h u_h^1)_{N_x - \frac{1}{2}} \right) = 0, \tag{18b}$$

$$-d_2 \frac{1}{2} \left((\nabla_{yh} u_h^2)_{i, -\frac{1}{2}} + (\nabla_{yh} u_h^2)_{i, \frac{1}{2}} \right) = Bi^M \left(H(u_i^1 + u_1^D) - u_{i,0}^2 \right), \tag{18c}$$

$$d_2 \frac{1}{2} \left((\nabla_{yh} u_h^2)_{i, N_y + \frac{1}{2}} + (\nabla_{yh} u_h^2)_{i, N_y - \frac{1}{2}} \right) = 0, \tag{18d}$$

$$-d_3 \frac{1}{2} \left((\nabla_{yh} u_h^3)_{i, -\frac{1}{2}} + (\nabla_{yh} u_h^3)_{i, \frac{1}{2}} \right) = 0, \tag{18e}$$

$$d_3 \frac{1}{2} \left((\nabla_{yh} u_h^3)_{i, N_y + \frac{1}{2}} + (\nabla_{yh} u_h^3)_{i, N_y - \frac{1}{2}} \right) = -\eta(u_{i,N_y}^3, u_i^4), \tag{18f}$$

and the initial conditions

$$\begin{aligned} u_h^1(0) &= \mathscr{P}_h^1 u_1^0, \quad u_h^2(0) = \mathscr{P}_h^2 u_2^0, \\ u_h^3(0) &= \mathscr{P}_h^2 u_3^0, \quad u_h^4(0) = \mathscr{P}_h^1 u_4^0, \end{aligned} \tag{19}$$

where $\mathscr{P}_h^1$ and $\mathscr{P}_h^2$ are suitable projection operators from Ω to Ω_h and from $\Omega \times Y$ to ω_h, respectively.

Remark 1. The boundary conditions (18b)–(18f) are a centered-difference approximation of conditions (3) and are written so as to stress the relation between the two. Using the definition of discrete ∇_h and ∇_{yh} operators, (18) can be rewritten in terms of auxiliary values of u_h^k, $k = 1, \ldots, 4$, on nodes outside the grids as follows:

$$u_0^1 = 0, \tag{20a}$$

$$u_{N_x+1}^1 = u_{N_x-1}^1, \tag{20b}$$

$$u_{i,-1}^2 = u_{i,1}^2 + \frac{2h_y}{d_2} Bi^M \left(H(u_i^1 + u_1^D) - u_{i,0}^2 \right), \tag{20c}$$

$$u_{i,N_y+1}^2 = u_{i,N_y-1}^2, \tag{20d}$$

$$u_{i,-1}^3 = u_{i,1}^3, \tag{20e}$$

$$u_{i,N_y+1}^3 = u_{i,N_y-1}^3 - \frac{2h_y}{d_3} \eta(u_{i,N_y}^3, u_i^4). \tag{20f}$$

Proposition 3. *Assume (A1)–(A4) to be fulfilled. Then there exists a unique semi-discrete solution*

$$\{u_h^1, u_h^2, u_h^3, u_h^4\} \in C^1([0,T]; \mathscr{G}_h) \times C^1([0,T]; \mathscr{F}_h) \times C^1([0,T]; \mathscr{G}_h) \times C^1([0,T]; \mathscr{F}_h)$$

in the sense of Definition 2.

Proof. The proof, based on the standard ode argument, follows in a straightforward manner. $\square$

3.4 Discrete scalar products and norms

Next, we introduce scalar products and norms on the spaces of grid functions $\mathscr{G}_h$, $\mathscr{E}_h$, $\mathscr{F}_h$, $\mathscr{G}_h$ and we show some basic integral identities for the difference operators.

Let $(\gamma_i^1)_{i=0}^{N_x}$ and $(\gamma_j^2)_{j=0}^{N_y}$ be such that

$$\gamma_i^1 := \begin{cases} 1 & 1 \le i \le N_x - 1, \\ \frac{1}{2} & i \in \{0, N_x\}, \end{cases}, \qquad \gamma_j^2 := \begin{cases} 1 & 1 \le j \le N_y - 1, \\ \frac{1}{2} & j \in \{0, N_y\}, \end{cases} \tag{21}$$

and define the following discrete L^2 scalar products and the corresponding discrete L^2 norms

$$(u_h, v_h)_{\mathscr{G}_h} := h_x \sum_{x_i \in \Omega_h} \gamma_i^1 u_i v_i, \qquad\qquad u_h, v_h \in \mathscr{G}_h, \tag{22}$$

$$\|u_h\|_{\mathscr{G}_h} := \sqrt{(u_h, u_h)_{\mathscr{G}_h}}, \qquad\qquad u_h \in \mathscr{G}_h, \tag{23}$$

$$(u_h, v_h)_{\mathscr{G}_h^o} := h_x \sum_{x_i \in \Omega_h^o} \gamma_i^1 u_i v_i, \qquad\qquad u_h, v_h \in \mathscr{G}_h^o, \tag{24}$$

$$\|u_h\|_{\mathscr{G}_h^o} := \sqrt{(u_h, u_h)_{\mathscr{G}_h^o}}, \qquad\qquad u_h \in \mathscr{G}_h^o, \tag{25}$$

$$(u_h, v_h)_{\mathscr{F}_h} := h_x h_y \sum_{x_{ij} \in \omega_h} \gamma_i^1 \gamma_j^2 u_{ij} v_{ij}, \qquad\qquad u_h, v_h \in \mathscr{F}_h, \tag{26}$$

$$\|u_h\|_{\mathscr{F}_h} := \sqrt{(u_h, u_h)_{\mathscr{F}_h}}, \qquad\qquad u_h \in \mathscr{F}_h, \tag{27}$$

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$$(\mathsf{u}_h, \mathsf{v}_h)_{\mathscr{E}_h} := h_x \sum_{x_{i+1/2} \in \Omega_h^e} \mathsf{u}_{i+1/2} \mathsf{v}_{i+1/2}, \qquad\qquad \mathsf{u}_h, \mathsf{v}_h \in \mathscr{E}_h, \tag{28}$$

$$\|\mathsf{u}_h\|_{\mathscr{E}_h} := \sqrt{(\mathsf{u}_h, \mathsf{u}_h)_{\mathscr{E}_h}}, \qquad\qquad \mathsf{u}_h \in \mathscr{E}_h, \tag{29}$$

$$(\mathsf{u}_h, \mathsf{v}_h)_{\mathscr{H}_h} := h_x h_y \sum_{x_{i,j+1/2} \in \omega_h^e} \gamma_i^1 \mathsf{u}_{i,j+1/2} \mathsf{v}_{i,j+1/2}, \qquad\qquad \mathsf{u}_h, \mathsf{v}_h \in \mathscr{H}_h, \tag{30}$$

$$\|\mathsf{u}_h\|_{\mathscr{H}_h} := \sqrt{(\mathsf{u}_h, \mathsf{u}_h)_{\mathscr{H}_h}}, \qquad\qquad \mathsf{u}_h \in \mathscr{H}_h. \tag{31}$$

It can be shown that a discrete equivalent of Green's formula holds for these scalar products as well as other identities as is stated in the following lemmas.

Lemma 4 (Discrete macro Green-like formula)**.** *Let $u_h \in \mathscr{G}_h$ and $\mathsf{v}_h \in \mathscr{E}_h$ such that*

$$u_0 = 0, \quad u_{N_x+1} = u_{N_x-1}, \tag{32}$$

$$\mathsf{v}_{N_x+1/2} = -\mathsf{v}_{N_x-1/2}. \tag{33}$$

Then the following identity holds:

$$(u_h, \mathrm{div}_h\, \mathsf{v}_h)_{\mathscr{G}_h^o} = -(\nabla_h u_h, \mathsf{v}_h)_{\mathscr{E}_h}. \tag{34}$$

Lemma 5 (Discrete micro-macro Green-like formula)**.** *Let $u_h \in \mathscr{F}_h$ and $\mathsf{v}_h \in \mathscr{H}_h$ such that*

$$-\frac{1}{2}\left(\mathsf{v}_{k,-1/2} + \mathsf{v}_{k,1/2}\right) = \delta_k^1, \quad \frac{1}{2}\left(\mathsf{v}_{k,N_y-1/2} + \mathsf{v}_{k,N_y+1/2}\right) = \delta_k^2, \tag{35}$$

$$u_{k,-1} = u_{k,1} + 2h_y \delta_k^1, \qquad u_{k,N_y+1} = u_{k,N_y-1} + 2h_y \delta_k^2, \tag{36}$$

for $i = 0, \dots, N_x$, and $\delta_h^1, \delta_h^2 \in \mathscr{G}_h$. Then the following identity holds:

$$(u_h, \mathrm{div}_{yh}\, \mathsf{v}_h)_{\mathscr{F}_h} = -(\nabla_{yh} u_h, \mathsf{v}_h)_{\mathscr{H}_h} + (u_h|_{y=0}, \delta_h^1)_{\mathscr{G}_h} + (u_h|_{y=N_y}, \delta_h^2)_{\mathscr{G}_h}. \tag{37}$$

We also frequently make use of the following discrete trace inequality:

Lemma 6 (Discrete trace inequality)**.** *For $u_h \in \mathscr{F}_h$ there exists a positive constant C depending only on Ω such that*

$$\|u_h|_{y=\ell}\|_{\mathscr{G}_h} \leq C(\|u_h\|_{\mathscr{F}_h} + \|\nabla_{yh} u_h\|_{\mathscr{H}_h}). \tag{38}$$

Proof. Our proof follows the line of thought of [10]. We have that for $u_h \in \mathscr{F}_h$

$$|u_{i,N_y}| \leq \sum_{j=0}^{N_y-1} |u_{i,j+1} - u_{ij}| + \sum_{j=0}^{N_y} \gamma_j^2 h_y |u_{ij}|.$$

Squaring both sides of the inequality, we get

$$(u_{i,N_y})^2 \leq A_i + B_i, \tag{39}$$

where

$$A_i := 2\left(\sum_{j=0}^{N_y-1} |u_{i,j+1} - u_{ij}|\right)^2 \quad \text{and } B_i := 2\left(\sum_{j=0}^{N_y} \gamma_j^2 h_y |u_{ij}|\right)^2.$$

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Applying the Cauchy-Schwarz inequality to A_i, we obtain

$$A_i \leq 2 \sum_{j=0}^{N_y-1} h_y \left(\frac{u_{i,j+1} - u_{ij}}{h_y} \right)^2 \sum_{j=0}^{N_y-1} h_y = 2\ell \sum_{j=0}^{N_y-1} h_y \left(\frac{u_{i,j+1} - u_{ij}}{h_y} \right)^2 .$$

Similarly, using the Cauchy-Schwarz inequality we get for B_i

$$B_i \leq 2 \sum_{j=0}^{N_y} \gamma_j^2 h_y (u_{ij})^2 \sum_{j=0}^{N_y} \gamma_j^2 h_y = 2\ell \sum_{j=0}^{N_y} \gamma_j^2 h_y (u_{ij})^2 .$$

Multiplying (39) by $\gamma_i^1 h_x$, summing over $i \in \{0, \dots, N_x\}$ and then using the bounds on A_i and B_i, it yields that:

$$\sum_{i=0}^{N_x} \gamma_i^1 h_x (u_{i,N_y})^2 \leq 2\ell \left(\sum_{i=0}^{N_x} \sum_{j=0}^{N_y-1} \gamma_i^1 h_x h_y \left((\nabla_{yh} u_h)_{i,j+\frac{1}{2}} \right)^2 + \sum_{x_{ij} \in \omega_h} \gamma_i^1 \gamma_j^2 h_x h_y (u_{ij})^2 \right),$$

that is

$$\| u_h|_{y=\ell} \|_{\mathscr{G}_h}^2 \leq C \left(\| \nabla_{yh} u_h \|_{\mathscr{H}_h}^2 + \| u_h \|_{\mathscr{F}_h}^2 \right),$$

from which the claim of the Lemma follows directly. $\qquad\square$

4 Approximation estimates

The aim of this section is to derive *a priori* estimates on the semi-discrete solution. Based on weak convergence-type arguments, the estimates will ensure, at least up to subsequences, a (weakly) convergent way to reconstruct the weak solution to problem (P).

4.1 *A priori* estimates

This is the place where we use the tools developed in section 3.

In subsequent paragraphs, we refer to the following relations: From scalar product of (17a) with $\varphi_h^1 \in \mathscr{G}_h$, (17b) and (17c) with $\varphi_h^2 \in \mathscr{F}_h$ and φ_h^3, respectively, and (17d) with $\varphi_h^4 \in \mathscr{G}_h$ to obtain

$$(\dot{u}_h^1, \varphi_h^1)_{\mathscr{G}_h^o} = d_1 (\Delta_h u_h^1, \varphi_h^1)_{\mathscr{G}_h^o} - Bi^M \left(Hu_h^1 - u_h^2|_{y=0}, \varphi_h^1 \right)_{\mathscr{G}_h^o}, \tag{40}$$

$$(\dot{u}_h^2, \varphi_h^2)_{\mathscr{F}_h} = d_2 (\Delta_{yh} u_h^2, \varphi_h^2)_{\mathscr{F}_h} - \alpha (u_h^2, \varphi_h^2)_{\mathscr{F}_h} + \beta (u_h^3, \varphi_h^2)_{\mathscr{F}_h}, \tag{41}$$

$$(\dot{u}_h^3, \varphi_h^3)_{\mathscr{F}_h} = d_3 (\Delta_{yh} u_h^3, \varphi_h^3)_{\mathscr{F}_h} + \alpha (u_h^2, \varphi_h^3)_{\mathscr{F}_h} - \beta (u_h^3, \varphi_h^3)_{\mathscr{F}_h}, \tag{42}$$

$$(\dot{u}_h^4, \varphi_h^4)_{\mathscr{G}_h} = \left(\eta (u_h^3|_{y=\ell}, u_h^4), \varphi_h^4 \right)_{\mathscr{G}_h}. \tag{43}$$

Note that u_h^1 and $\nabla_h \varphi_h^1$ satisfy the assumptions of Lemma 4, u_h^2 and $\nabla_{yh} \varphi_h^2$ satisfy the assumptions of Lemma 5 with $\delta_k^1 = \frac{Bi^M}{d_2} (Hu_k^1 - u_{k,0}^2)$ and $\delta_k^2 = 0$, and u_h^3 and $\nabla_{yh} \varphi_h^3$ with $\delta_k^1 = 0$ and $\delta_k^2 = -\frac{1}{d_3} \eta (u_{k,N_y}^3, u_k^4)$. Thus, using Lemmas 4, 5 and properties of the discrete scalar products we get

$$(\dot{u}_h^1, \varphi_h^1)_{\mathscr{G}_h} + d_1 (\nabla_h u_h^1, \nabla_h \varphi_h^1)_{\mathscr{E}_h} = -Bi^M \left(Hu_h^1 - u_h^2|_{y=0}, \varphi_h^1 \right)_{\mathscr{G}_h}, \tag{44}$$

$$(\dot{u}_h^2, \varphi_h^2)_{\mathscr{F}_h} + d_2 (\nabla_{yh} u_h^2, \nabla_{yh} \varphi_h^2)_{\mathscr{H}_h} = Bi^M (Hu_h^1 - u_h^2|_{y=0}, \varphi_h^2|_{y=0})_{\mathscr{G}_h} - \alpha (u_h^2, \varphi_h^2)_{\mathscr{F}_h} + \beta (u_h^3, \varphi_h^2)_{\mathscr{F}_h}, \tag{45}$$

$$(\dot{u}_h^3, \varphi_h^3)_{\mathscr{F}_h} + d_3 (\nabla_{yh} u_h^3, \nabla_{yh} \varphi_h^3)_{\mathscr{H}_h} = -\left(\eta (u_h^3|_{y=\ell}, u_h^4), \varphi_h^3|_{y=\ell} \right)_{\mathscr{G}_h} + \alpha (u_h^2, \varphi_h^3)_{\mathscr{F}_h} - \beta (u_h^3, \varphi_h^3)_{\mathscr{F}_h}, \tag{46}$$

$$(\dot{u}_h^4, \varphi_h^4)_{\mathscr{G}_h} = \left(\eta (u_h^3|_{y=\ell}, u_h^4), \varphi_h^4 \right)_{\mathscr{G}_h}. \tag{47}$$

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Lemma 7 (Discrete energy estimates). *Let $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ be a semi-discrete solution of (2) for some $T > 0$. Then it holds that*

$$\max_{t \in S} \left(\|u_h^1(t)\|_{\mathscr{G}_h}^2 + \|u_h^2(t)\|_{\mathscr{F}_h}^2 + \|u_h^3(t)\|_{\mathscr{F}_h}^2 + \|u_h^4(t)\|_{\mathscr{G}_h}^2 \right) \leq C, \tag{48}$$

$$\int_0^T \left(\|\nabla_h u_h^1\|_{\mathscr{E}_h}^2 + \|\nabla_{yh} u_h^2\|_{\mathscr{H}_h}^2 + \|\nabla_{yh} u_h^3\|_{\mathscr{H}_h}^2 \right) \mathrm{d}t \leq C, \tag{49}$$

where $C := \bar{C}\left(\|u_h^1(0)\|_{\mathscr{G}_h}^2 + \|u_h^2(0)\|_{\mathscr{F}_h}^2 + \|u_h^3(0)\|_{\mathscr{F}_h}^2 + \|u_h^4(0)\|_{\mathscr{G}_h}^2 \right)$, with $\bar{C}$ being a positive constant independent of h_x, h_y.

Proof. In (44)–(47), taking $(\varphi_h^1, \varphi_h^2, \varphi_h^3, \varphi_h^4) = (u_h^1, u_h^2, u_h^3, u_h^4)$, summing the equalities, applying Young's inequality on terms with $(u_h^2, u_h^3)_{\mathscr{F}_h}$, dropping the negative terms on the right-hand side, and multiplying the resulting inequality by 2 give

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\|u_h^1\|_{\mathscr{G}_h}^2 + \|u_h^2\|_{\mathscr{F}_h}^2 + \|u_h^3\|_{\mathscr{F}_h}^2 + \|u_h^4\|_{\mathscr{G}_h}^2 \right) + 2d_1 \|\nabla_h u_h^1\|_{\mathscr{E}_h}^2 + 2d_2 \|\nabla_{yh} u_h^2\|_{\mathscr{H}_h}^2 + 2d_3 \|\nabla_{yh} u_h^3\|_{\mathscr{H}_h}^2$$

$$\leq -2Bi^M (Hu_h^1 - u_h^2|_{y=0}, u_h^1)_{\mathscr{G}_h} + 2Bi^M (Hu_h^1 - u_h^2|_{y=0}, u_h^2|_{y=0})_{\mathscr{G}_h}$$

$$+ C_1 \|u_h^2\|_{\mathscr{F}_h}^2 + C_1 \|u_h^3\|_{\mathscr{F}_h}^2 + 2\left(\eta(u_h^3|_{y=\ell}, u_h^4), u_h^4 - u_h^3|_{y=\ell} \right)_{\mathscr{G}_h},$$

where $C_1 := \alpha + \beta > 0$. Expanding the first two terms on the right-hand side we get

$$-2(Hu_h^1 - u_h^2|_{y=0}, u_h^1)_{\mathscr{G}_h} + 2(Hu_h^1 - u_h^2|_{y=0}, u_h^2|_{y=0})_{\mathscr{G}_h} = -2H \|u_h^1\|_{\mathscr{G}_h}^2$$

$$+ 2(1+H)(u_h^1, u_h^2|_{y=0})_{\mathscr{G}_h} - 2\|u_h^2|_{y=0}\|_{\mathscr{G}_h}^2 \leq \frac{1+H}{\varepsilon} \|u_h^1\|_{\mathscr{G}_h}^2 + \left((1+H)\varepsilon - 2 \right) \|u_h^2|_{y=0}\|_{\mathscr{G}_h}^2,$$

where we used Young's inequality with $\varepsilon > 0$. Choosing ε sufficiently small, the coefficient in front of the last term is negative, so we have that

$$-2(Hu_h^1 - u_h^2|_{y=0}, u_h^1)_{\mathscr{G}_h} + 2(Hu_h^1 - u_h^2|_{y=0}, u_h^2|_{y=0})_{\mathscr{G}_h} \leq C_2 \|u_h^1\|_{\mathscr{G}_h}^2,$$

where $C_2 := \frac{1+H}{\varepsilon} > 0$, and thus

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\|u_h^1\|_{\mathscr{G}_h}^2 + \|u_h^2\|_{\mathscr{F}_h}^2 + \|u_h^3\|_{\mathscr{F}_h}^2 + \|u_h^4\|_{\mathscr{G}_h}^2 \right) + 2d_1 \|\nabla_h u_h^1\|_{\mathscr{E}_h}^2 + 2d_2 \|\nabla_{yh} u_h^2\|_{\mathscr{H}_h}^2 + 2d_3 \|\nabla_{yh} u_h^3\|_{\mathscr{H}_h}^2$$

$$\leq C_2 \|u_h^1\|_{\mathscr{G}_h}^2 + C_1 \|u_h^2\|_{\mathscr{F}_h}^2 + C_1 \|u_h^3\|_{\mathscr{F}_h}^2 + 2\left(\eta(u_h^3|_{y=\ell}, u_h^4), u_h^4 - u_h^3|_{y=\ell} \right)_{\mathscr{G}_h}. \tag{50}$$

For the last term on the right-hand side of the previous inequality we have

$$2\left(\eta(u_h^3|_{y=\ell}, u_h^4), u_h^4 - u_h^3|_{y=\ell} \right)_{\mathscr{G}_h} = 2k \left(R(u_h^3|_{y=\ell})Q(u_h^4), u_h^4 \right)_{\mathscr{G}_h} \underbrace{-2k \left(R(u_h^3|_{y=\ell})Q(u_h^4), u_h^3|_{y=\ell} \right)_{\mathscr{G}_h}}_{\leq 0}$$

$$\leq 2k\bar{c}^q \left(R(u_h^3|_{y=\ell}), u_h^4 \right)_{\mathscr{G}_h} \leq k\bar{c}^q \left(\varepsilon \|R(u_h^3|_{y=\ell})\|_{\mathscr{G}_h}^2 + \frac{1}{\varepsilon} \|u_h^4\|_{\mathscr{G}_h}^2 \right) \leq k\bar{c}^q \left(\varepsilon \|u_h^3|_{y=\ell}\|_{\mathscr{G}_h}^2 + \frac{1}{\varepsilon} \|u_h^4\|_{\mathscr{G}_h}^2 \right)$$

$$\leq k\bar{c}^q \left(C_3 \varepsilon \|u_h^3\|_{\mathscr{F}_h}^2 + C_3 \varepsilon \|\nabla_{yh} u_h^3\|_{\mathscr{H}_h}^2 + \frac{1}{\varepsilon} \|u_h^4\|_{\mathscr{G}_h}^2 \right),$$

where we used the assumption (A_1), Young's inequality with $\varepsilon > 0$ and the discrete trace inequality (38) with the constant $C_3 > 0$. Using the result in (50) we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\|u_h^1\|_{\mathscr{G}_h}^2 + \|u_h^2\|_{\mathscr{F}_h}^2 + \|u_h^3\|_{\mathscr{F}_h}^2 + \|u_h^4\|_{\mathscr{G}_h}^2 \right) + d_1 \|\nabla_h u_h^1\|_{\mathscr{E}_h}^2 + d_2 \|\nabla_{yh} u_h^2\|_{\mathscr{H}_h}^2 + C_4 \|\nabla_{yh} u_h^3\|_{\mathscr{H}_h}^2$$

$$\leq C_2 \|u_h^1\|_{\mathscr{G}_h}^2 + C_1 \|u_h^2\|_{\mathscr{F}_h}^2 + C_5 \|u_h^3\|_{\mathscr{F}_h}^2 + C_6 \|u_h^4\|_{\mathscr{G}_h}^2, \tag{51}$$

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where $C_4 := d_3 - k\bar{c}^q C_3 \varepsilon$ can be made positive for ε sufficiently small, $C_5 := C_1 + k\bar{c}^q C_3 \varepsilon$, and $C_6 := k\bar{c}^q \frac{1}{\varepsilon}$.

Discarding the terms with discrete gradient, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\|u_h^1\|_{\mathscr{G}_h}^2 + \|u_h^2\|_{\mathscr{F}_h}^2 + \|u_h^3\|_{\mathscr{F}_h}^2 + \|u_h^4\|_{\mathscr{G}_h}^2\right) \leq C_7\left(\|u_h^1\|_{\mathscr{G}_h}^2 + \|u_h^2\|_{\mathscr{F}_h}^2 + \|u_h^3\|_{\mathscr{F}_h}^2 + \|u_h^4\|_{\mathscr{G}_h}^2\right),$$

where $C_7 := \max\{C_1, C_2, C_5, C_6\}$. Applying the Gronwall's lemma to the previous inequality we obtain

$$\max_{t \in S}\left(\|u_h^1(t)\|_{\mathscr{G}_h}^2 + \|u_h^2(t)\|_{\mathscr{F}_h}^2 + \|u_h^3(t)\|_{\mathscr{F}_h}^2 + \|u_h^4(t)\|_{\mathscr{G}_h}^2\right)$$
$$\leq \left(\|u_h^1(0)\|_{\mathscr{G}_h}^2 + \|u_h^2(0)\|_{\mathscr{F}_h}^2 + \|u_h^3(0)\|_{\mathscr{F}_h}^2 + \|u_h^4(0)\|_{\mathscr{G}_h}^2\right)e^{C_7 T}. \quad (52)$$

Finally, integrating (51) over $[0, T]$ and using (52) gives

$$\int_0^T \left(\|\nabla_h u_h^1\|_{\mathscr{E}_h}^2 + \|\nabla_{yh} u_h^2\|_{\mathscr{H}_h}^2 + \|\nabla_{yh} u_h^3\|_{\mathscr{H}_h}^2\right)\mathrm{d}t$$
$$\leq \frac{1 + C_7 T e^{C_7 T}}{C_8}\left(\|u_h^1(0)\|_{\mathscr{G}_h}^2 + \|u_h^2(0)\|_{\mathscr{F}_h}^2 + \|u_h^3(0)\|_{\mathscr{F}_h}^2 + \|u_h^4(0)\|_{\mathscr{G}_h}^2\right), \quad (53)$$

where $C_8 := \min\{d_1, d_2, C_4\}$. The claim of the lemma directly follows. □

Lemma 8. *Let* $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ *be a semi-discrete solution of* (2) *for some* $T > 0$. *Then it holds that*

$$\max_{t \in S}\left(\|\dot{u}_h^1(t)\|_{\mathscr{G}_h}^2 + \|\dot{u}_h^2(t)\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3(t)\|_{\mathscr{F}_h}^2\right) \leq C, \quad (54)$$

$$\int_0^T \left(\|\nabla_h \dot{u}_h^1\|_{\mathscr{E}_h}^2 + \|\nabla_{yh} \dot{u}_h^2\|_{\mathscr{H}_h}^2 + \|\nabla_{yh} \dot{u}_h^3\|_{\mathscr{H}_h}^2\right)\mathrm{d}t \leq C, \quad (55)$$

where C *is a positive constant independent of* h_x, h_y.

Proof. We follow the steps of [19, Theorem 4]. Differentiate (44)–(46) with respect to time, take $\varphi_h^i = \dot{u}_h^i, i = 1, \dots, 3$, discard the negative terms on the right-hand side and sum the inequalities to obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|\dot{u}_h^1\|_{\mathscr{G}_h}^2 + \|\dot{u}_h^2\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3\|_{\mathscr{F}_h}^2\right) + d_1\|\nabla_h \dot{u}_h^1\|_{\mathscr{E}_h}^2 + d_2\|\nabla_{yh} \dot{u}_h^2\|_{\mathscr{H}_h}^2 + d_3\|\nabla_{yh} \dot{u}_h^3\|_{\mathscr{H}_h}^2$$
$$\leq Bi^M(1+H)\left(\dot{u}_h^1, \dot{u}_h^2|_{y=0}\right)_{\mathscr{G}_h} - Bi^M\|\dot{u}_h^2|_{y=0}\|_{\mathscr{G}_h}^2 + (\alpha+\beta)\left(\dot{u}_h^2, \dot{u}_h^3\right)_{\mathscr{F}_h}$$
$$- \left(\partial_r \eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^3|_{y=\ell} + \partial_s \eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^4, \dot{u}_h^3|_{y=\ell}\right)_{\mathscr{G}_h}.$$

As in the proof of Lemma 7, for the first two terms on the right-hand side we have that

$$Bi^M(1+H)\left(\dot{u}_h^1, \dot{u}_h^2|_{y=0}\right)_{\mathscr{G}_h} - Bi^M\|\dot{u}_h^2|_{y=0}\|_{\mathscr{G}_h}^2 \leq C_1\|\dot{u}_h^1\|_{\mathscr{G}_h}^2,$$

and for the third term

$$(\alpha+\beta)\left(\dot{u}_h^2, \dot{u}_h^3\right)_{\mathscr{F}_h} \leq C_2\left(\|\dot{u}_h^2\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3\|_{\mathscr{F}_h}^2\right).$$

Using the Lipschitz property of η, together with Schwarz's and Young's inequalities, and assuming the structural restriction $\partial_r \eta > 0$, we obtain for the last term on the right-hand side that

$$- \left(\partial_r \eta \dot{u}_h^3|_{y=\ell} + \partial_s \eta \dot{u}_h^4|_{y=\ell}, \dot{u}_h^3|_{y=\ell}\right)_{\mathscr{G}_h} = -\left(\partial_r \eta \dot{u}_h^3|_{y=\ell}, \dot{u}_h^3|_{y=\ell}\right)_{\mathscr{G}_h} - \left(\partial_s \eta \dot{u}_h^4|_{y=\ell}, \dot{u}_h^3|_{y=\ell}\right)_{\mathscr{G}_h}$$
$$\leq \underbrace{-\left(\partial_r \eta \dot{u}_h^3|_{y=\ell}, \dot{u}_h^3|_{y=\ell}\right)_{\mathscr{G}_h}}_{\leq 0} + C\left(\frac{1}{2\varepsilon}\|\dot{u}_h^4\|_{\mathscr{G}_h}^2 + \frac{\varepsilon}{2}\|\dot{u}_h^3|_{y=\ell}\|_{\mathscr{G}_h}^2\right).$$

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Choosing ε sufficiently small, we get that

$$-\left(\partial_r \eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^3|_{y=\ell} + \partial_s \eta(u_h^3|_{y=\ell}, u_h^4)\dot{u}_h^4, \dot{u}_h^3|_{y=\ell}\right)_{\mathscr{G}_h} \leq C_3 \left\| \dot{u}_h^4 \right\|_{\mathscr{G}_h}^2.$$

Putting the obtained results together we finally obtain that

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(\|\dot{u}_h^1\|_{\mathscr{G}_h}^2 + \|\dot{u}_h^2\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3\|_{\mathscr{F}_h}^2\right) + d_1\|\nabla_h \dot{u}_h^1\|_{\mathscr{E}_h}^2 + d_2\|\nabla_{yh}\dot{u}_h^2\|_{\mathscr{H}_h}^2 + d_3\|\nabla_{yh}\dot{u}_h^3\|_{\mathscr{H}_h}^2$$
$$\leq C_1\|\dot{u}_h^1\|_{\mathscr{G}_h}^2 + C_2\left(\|\dot{u}_h^2\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3\|_{\mathscr{F}_h}^2\right) + C_3\|\dot{u}_h^4\|_{\mathscr{G}_h}^2. \quad (56)$$

Grönwall's inequality gives that

$$\max_{t \in S}\left(\|\dot{u}_h^1\|_{\mathscr{G}_h}^2 + \|\dot{u}_h^2\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3\|_{\mathscr{F}_h}^2\right) \leq C_4\left(\|\dot{u}_h^1(0)\|_{\mathscr{G}_h}^2 + \|\dot{u}_h^2(0)\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3(0)\|_{\mathscr{F}_h}^2\right). \quad (57)$$

In order to estimate the right-hand side in the previous inequality, we evaluate (40)–(42) at $t = 0$ and test with $\left(\dot{u}_h^1(0), \dot{u}_h^2(0), \dot{u}_h^3(0)\right)$ to get

$$\|\dot{u}_h^1(0)\|_{\mathscr{G}_h}^2 + \|\dot{u}_h^2(0)\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3(0)\|_{\mathscr{F}_h}^2 = d_1(\Delta_h u_h^1(0), \dot{u}_h^1(0))_{\mathscr{G}_h^o} + d_2(\Delta_{yh}u_h^2(0), \dot{u}_h^2(0))_{\mathscr{F}_h}$$
$$+ d_3(\Delta_{yh}u_h^3(0), \dot{u}_h^3(0))_{\mathscr{F}_h} - Bi^M\left(Hu_h^1(0) - u_h^2(0)|_{y=0}, \dot{u}_h^1(0)\right)_{\mathscr{G}_h}$$
$$+ (\alpha u_h^2(0) - \beta u_h^3(0), \dot{u}_h^3(0) - \dot{u}_h^2(0))_{\mathscr{F}_h}.$$

Schwarz's inequality and Young's inequality (with $\varepsilon > 0$ chosen sufficiently small) together with the regularity of the initial data yield the estimate

$$\|\dot{u}_h^1(0)\|_{\mathscr{G}_h}^2 + \|\dot{u}_h^2(0)\|_{\mathscr{F}_h}^2 + \|\dot{u}_h^3(0)\|_{\mathscr{F}_h}^2 \leq C,$$

where C does not depend on the spatial step sizes. Returning back to (56), integrating it with respect to t and using (57) gives the claim of the lemma. $\qquad\square$

In the following lemma we derive additional *a priori* estimates that will finally allow us to pass in the limit in the non-linear terms. In order to avoid introducing new grids, grid functions and associated scalar products for finite differences in x variable, we will resort to sum notation in this proof. To this end, for $u_h \in \mathscr{F}_h$, let $\delta_x^+ u_{ij}$, $\delta_x^- u_{ij}$, $\delta_y^+ u_{ij}$, $\delta_y^- u_{ij}$ denote the forward and backward difference quotients at x_{ij} in x- and y-direction, i.e.,

$$(\delta_x^+ u_h)_{ij} := \frac{u_{i+1,j} - u_{ij}}{h_x}, \quad (\delta_x^- u_h)_{ij} := \frac{u_{ij} - u_{i-1,j}}{h_x},$$
$$(\delta_y^+ u_h)_{ij} := \frac{u_{i,j+1} - u_{ij}}{h_y}, \quad (\delta_y^- u_h)_{ij} := \frac{u_{ij} - u_{i,j-1}}{h_y}.$$

Lemma 9 (Improved *a priori* estimates). *Let $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ be a semi-discrete solution of (2) for some $T > 0$. Then it holds that*

$$\max_{t \in S}\left(h_x h_y \sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\delta_x^+ u_{ij}^2)^2 + h_x h_y \sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\delta_x^+ u_{ij}^3)^2\right) \leq C, \quad (58)$$

$$\int_0^T h_x h_y \sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\delta_x^+ \delta_y^+ u_{ij}^2)^2\,\mathrm{d}t + \int_0^T h_x h_y \sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\delta_x^+ \delta_y^+ u_{ij}^3)^2\,\mathrm{d}t \leq C, \quad (59)$$

where C is a positive constant independent of h_x, h_y.

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Proof. Following the steps of [19, Theorem 5], introduce a function $\vartheta \in C_0^\infty(\Omega)$ such that $0 \le \vartheta \le 1$ and let $\vartheta_h := \vartheta|_{\Omega_h} \in \mathscr{G}_h$. Test (17b) with $-\delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{ij}$, (17c) with $-\delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{ij}$, and sum over ω_h to form relations analogous to (45), (46). We get

$$
-h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 \dot{u}_{ij}^2 \delta_x^-(\vartheta_h^2 \delta_x^+ u_h^2)_{ij} - d_2 h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y-1} \gamma_i^1 \gamma_j^2 \delta_y^+ u_{ij}^2 \delta_y^+ (\delta_x^-(\vartheta_h^2 \delta_x^+ u_h^2))_{ij}
$$
$$
= -Bi^m \sum_{i=1}^{N_x} \gamma_i^1 (Hu_i^1 - u_{i,0}^2) \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{i,0} + \alpha h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^2 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{ij}
$$
$$
- \beta h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^3 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^2)_{ij},
$$

$$
-h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 \dot{u}_{ij}^3 \delta_x^-(\vartheta_h^2 \delta_x^+ u_h^3)_{ij} - d_3 h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y-1} \gamma_i^1 \gamma_j^2 \delta_y^+ u_{ij}^3 \delta_y^+ (\delta_x^-(\vartheta_h^2 \delta_x^+ u_h^3))_{ij}
$$
$$
= \sum_{i=1}^{N_x} \gamma_i^1 \eta(u_{i,N_y}^3, u_i^4) \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{i,N_y} - \alpha h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^2 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{ij}
$$
$$
+ \beta h_y \sum_{i=1}^{N_x} \sum_{j=0}^{N_y} \gamma_i^1 \gamma_j^2 u_{ij}^3 \delta_x^-(\vartheta_i^2 \delta_x^+ u_h^3)_{ij}.
$$

Summing the previous two equalities and using the discrete Green's theorem analogous to (34), Schwarz's inequality and Young's inequality we obtain

$$
\frac{1}{2} \frac{d}{dt} \left(h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y} |\vartheta_i \delta_x^+ u_{ij}^2|^2 + h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y} |\vartheta_i \delta_x^+ u_{ij}^3|^2 \right) + d_2 h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} |\vartheta_i \delta_x^+ \delta_y^+ u_{ij}^2|^2
$$
$$
+ d_3 h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y-1} |\vartheta_i \delta_x^+ \delta_y^+ u_{ij}^3|^2 \le Bi^m HC_1 \sum_{i=0}^{N_x-1} |\vartheta_i \delta_x^+ u_i^1|^2 + C_2 h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y} (\vartheta_i \delta_x^+ u_{ij}^2)^2
$$
$$
+ C_3 h_y \sum_{i=0}^{N_x-1} \sum_{j=0}^{N_y} (\vartheta_i \delta_x^+ u_{ij}^3)^2 - \sum_{i=0}^{N_x-1} (\delta_x^+ \eta(u_{i,N_y}^3, u_i^4))(\vartheta_i^2 \delta_x^+ u_{i,N_y}^3). \quad (60)
$$

We rewrite the last term on the right-hand side as

$$
-k \sum_{i=0}^{N_x-1} (\delta_x^+ (R(u_{i,N_y}^3) Q(u_i^4)))(\vartheta_i^2 \delta_x^+ u_{i,N_y}^3)
$$
$$
= -k \sum_{i=0}^{N_x-1} \left(Q(u_i^4) \delta_x^+ R(u_{i,N_y}^3) + R(u_{i+1,N_y}^3) \delta_x^+ Q(u_i^4) \right) (\vartheta_i^2 \delta_x^+ u_{i,N_y}^3)
$$
$$
= \underbrace{-k \sum_{i=0}^{N_x-1} \vartheta_i^2 Q(u_i^4) \delta_x^+ R(u_{i,N_y}^3) \delta_x^+ u_{i,N_y}^3}_{\le 0} - k \sum_{i=0}^{N_x-1} R(u_{i+1,N_y}^3) \delta_x^+ Q(u_i^4)(\vartheta_i^2 \delta_x^+ u_{i,N_y}^3),
$$

where we used the monotonicity of R and boundedness of Q. To estimate the last term we exploit the

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Lipschitz continuity and boundedness of Q and use the discrete trace theorem so that

$$-k\sum_{i=0}^{N_x-1} R(u_{i+1,N_y}^3)\delta_x^+ Q(u_i^4)(\vartheta_i^2\delta_x^+ u_{i,N_y}^3) \le C_4\sum_{i=0}^{N_x-1}\vartheta_i^2|\delta_x^+ u_{i,N_y}^3\delta_x^+ u_i^4|$$

$$\le \frac{C_4\varepsilon}{2}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+ u_{i,N_y}^3)^2 + \frac{C_4}{2\varepsilon}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+ u_i^4)^2 \le C_5\varepsilon h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+ u_{ij}^3)^2$$

$$+ C_5\varepsilon h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\vartheta_i\delta_x^+\delta_y^+ u_{ij}^3)^2 + \frac{C_4}{2\varepsilon}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+ u_i^4)^2.$$

Using the latter result in (60), we arrive at

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\left(h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+ u_{ij}^2)^2 + h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+ u_{ij}^3)^2\right) + d_2 h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\vartheta_i\delta_x^+\delta_y^+ u_{ij}^2)^2$$

$$+ (d_3 - C_5\varepsilon)h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y-1}(\vartheta_i\delta_x^+\delta_y^+ u_{ij}^3)^2 \le Bi^m HC_1\sum_{i=0}^{N_x-1}|\vartheta_i\delta_x^+ u_i^1|^2 + C_2 h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+ u_{ij}^2)^2$$

$$+ (C_3 + C_5\varepsilon)h_y\sum_{i=0}^{N_x-1}\sum_{j=0}^{N_y}(\vartheta_i\delta_x^+ u_{ij}^3)^2 + \frac{C_4}{2\varepsilon}\sum_{i=0}^{N_x-1}(\vartheta_i\delta_x^+ u_i^4)^2. \quad (61)$$

Applying Gronwall's inequality and integrating with respect to time we obtain the claim of the lemma. $\qquad\square$

5 Interpolation and compactness

In this section, we derive sufficient results that enable us to show the convergence of semi-discrete solutions of (2). To this end, we firstly introduce extensions of grid functions so that they are defined almost everywhere in Ω and ω and can be studied by the usual techniques of Lebesgue/Sobolev/Bochner spaces. Finally, we use the *a priori* estimates proved in section 4 to show the necessary compactness for the sequences of extended grid functions.

5.1 Interpolation

In this subsection we introduce extensions of grid functions so that they are defined almost everywhere in Ω and ω.

Definition 10 (Dual and simplicial grids on Ω). Let Ω_h be a grid on Ω as defined in Section 3.1. Define the dual grid $\Omega_h^\square$ as

$$\Omega_h^\square := \{\mathscr{K}_i^\square \subset \bar\Omega \mid \mathscr{K}_i^\square := [x_i - h_x/2, x_i + h_x/2]\cap\bar\Omega, \; x_i\in\Omega_h\},$$

and the simplicial grid $\Omega_h^\triangle$ as

$$\Omega_h^\triangle := \{\mathscr{K}_i^\triangle \subset \bar\Omega \mid \mathscr{K}_i^\triangle := [x_i, x_{i+1}]\cap\bar\Omega, \; x_i\in\Omega_h\}.$$

Definition 11 (Dual and simplicial grids on $\Omega\times Y$). Let ω_h be a grid on $\Omega\times Y$ as defined in Section 3.1. Define the dual grid $\omega_h^\square$ as

$$\omega_h^\square := \{\mathscr{L}_{ij}^\square \subset \bar\Omega\times\bar Y \mid \mathscr{L}_{ij}^\square := [x_i - h_x/2, x_i + h_x/2]$$

$$\times [y_j - h_y/2, y_j + h_y/2]\cap\bar\Omega\times\bar Y, \; x_i\in\Omega_h, y_j\in Y_h\},$$

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and the simplicial grid $\omega_h^{\boxbslash}$ as $\omega_h^{\boxbslash} := \omega_h^{\triangleleft} \cup \omega_h^{\triangleright}$, where

$$\omega_h^{\triangleleft} := \left\{ \mathscr{L}_{ij}^{\triangleleft} \mid \mathscr{L}_{ij}^{\triangleleft} := \left[(x_i, y_j), (x_{i+1}, y_j), (x_i, y_{j+1}) \right]_{\varkappa} \cap \bar{\Omega} \times \bar{Y}, i = 0, \ldots, N_x - 1, j = 0, \ldots, N_y - 1 \right\},$$

$$\omega_h^{\triangleright} := \left\{ \mathscr{L}_{ij}^{\triangleright} \mid \mathscr{L}_{ij}^{\triangleright} := \left[(x_{i+1}, y_{j+1}), (x_{i+1}, y_j), (x_i, y_{j+1}) \right]_{\varkappa} \cap \bar{\Omega} \times \bar{Y}, i = 0, \ldots, N_x - 1, j = 0, \ldots, N_y - 1 \right\},$$

where $[x, y, z]_{\varkappa}$ denotes convex hull of points $x, y, z \in \mathbb{R}^2$.

Definition 12 (Piecewise constant extension). For a grid function u_h we define its piecewise constant extension $\bar{u}_h$ as

$$\bar{u}_h(x) = \begin{cases} u_i, & x \in \mathscr{K}_i^{\square}, \ u_h \in \mathscr{G}_h, \\ u_{ij}, & x \in \mathscr{L}_{ij}^{\square}, \ u_h \in \mathscr{F}_h. \end{cases} \tag{62}$$

Definition 13 (Piecewise linear extension). For a grid function $u_h \in \mathscr{G}_h$ we define its piecewise linear extension $\hat{u}_h$ as

$$\hat{u}_h(x) = u_i + (\nabla_h u_h)_{i+1/2}(x - x_i), \quad x \in \mathscr{K}_i^{\boxbslash}, \ u_h \in \mathscr{G}_h, \tag{63}$$

while for $u_h \in \mathscr{F}_h$ we define it as

$$\hat{u}_h(x) = \begin{cases} u_{ij} + \delta_x^+ u_{ij}(x - x_i) + (\nabla_{yh} u_h)_{i, j+1/2}(y - y_j), & x \in \mathscr{L}_{ij}^{\triangleleft}, \\ u_{i+1, j+1} + \delta_x^+ u_{i, j+1}(x_{i+1} - x) + (\nabla_{yh} u_h)_{i+1, j+1/2}(y_j - y), & x \in \mathscr{L}_{ij}^{\triangleright}. \end{cases} \tag{64}$$

The following lemma shows the relation between discrete scalar products of grid functions and scalar products of interpolated grid functions in $L^2(\Omega)$ and $L^2(\Omega \times Y)$ and follows by a direct calculation.

Lemma 14. *It holds that*

$$\begin{aligned} (\bar{u}_h, \bar{v}_h)_{L^2(\Omega)} &= (u_h, u_h)_{\mathscr{G}_h}, & u_h, v_h \in \mathscr{G}_h, \\ (\nabla \hat{u}_h, \nabla \hat{v}_h)_{L^2(\Omega)} &= (\nabla_h u_h, \nabla_h v_h)_{\mathscr{E}_h}, & u_h, v_h \in \mathscr{G}_h, \\ (\bar{u}_h, \bar{v}_h)_{L^2(\Omega \times Y)} &= (u_h, v_h)_{\mathscr{F}_h}, & u_h, v_h \in \mathscr{F}_h, \\ (\nabla_y \hat{u}_h, \nabla_y \hat{v}_h)_{L^2(\Omega \times Y)} &= (\nabla_{yh} u_h, \nabla_{yh} v_h)_{\mathscr{H}_h}, & u_h, v_h \in \mathscr{F}_h. \end{aligned}$$

5.2 Compactness

In this subsection we prove our main result. To do this we essentially use the preliminary results shown in the previous paragraphs and the results of [13]. Basically, we show the convergence of semi-discrete solutions to a weak solution of problem (P). This result is stated in the following theorem.

Theorem 15. *Assume (A1)–(A4) to be fulfilled. Then the semi-discrete solution $\{u_h^1, u_h^2, u_h^3, u_h^4\}$ of (2) exists on $[0, T]$ for any $T > 0$ and its interpolate $\{\hat{u}_h^1, \hat{u}_h^2, \hat{u}_h^3, \hat{u}_h^4\}$ converge in $L^2(\Omega)$, $L^2(\Omega \times Y)$, $L^2(\Omega \times S)$, $L^2(\Omega)$, respectively, as $|h| \to 0$ to a weak solution (u_1, u_2, u_3, u_4) to problem (P) in the sense of Definition 1.*

Proof. We start off with recovering the initial data. The definition of interpolation of grid functions leads, as $|h| \to 0$, to

$$\begin{aligned} \hat{u}_h^1(0) &\to u_1^0 \text{ weakly in } H^1(\Omega), \\ \hat{u}_h^2(0) &\to u_2^0 \text{ weakly in } L^2(\Omega; H^1(Y)), \\ \hat{u}_h^3(0) &\to u_3^0 \text{ weakly in } L^2(\Omega; H^1(Y)), \\ \hat{u}_h^4(0) &\to u_4^0 \text{ weakly in } L^2(\Omega). \end{aligned}$$

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Let h_n be a sequence of spatial space sizes such that $|h| \to 0$ as $n \to \infty$. Consequently, we obtain a sequence of solutions $\{u_{h_n}^1, u_{h_n}^2, u_{h_n}^3, u_{h_n}^4\}$ of (17) defined on the whole time interval S.

Let us pass to the limit $|h| \to 0$ in the ODE. Note that $\eta(\bar{u}_{h_n}^3|_{y=\ell}, \bar{u}_{h_n}^4) \rightharpoonup q$ weakly in $L^2(S; L^2(\Omega))$, and q still needs to be identified. The way we pass to the limit in the ODE is based on the following monotonicity-type argument (see [21]): using the monotonicity of η w.r.t. both variables, we can show that $\bar{u}_{h_n}^4$ is a Cauchy sequence, and therefore, it is strongly convergent to u^4.

Now, it only remains to pass to the limit in the PDEs. Note that the weak formulation contains a nonlinear boundary term involving $\eta(\cdot, \cdot)$. Exploiting the properties of the interpolations of grid functions we deduce that the same *a priori* estimates hold also for the interpolated solution (see also [13]). On this way, we obtain

$$\{\hat{u}_{h_n}^1\} \text{ is bounded in } L^\infty(0, T; L^2(\Omega)),$$
$$\{\hat{u}_{h_n}^1\} \text{ is bounded in } L^2(0, T; H^1(\Omega)),$$
$$\{\hat{u}_{h_n}^2\} \text{ is bounded in } L^\infty(0, T; L^2(\Omega)),$$
$$\{\hat{u}_{h_n}^3\} \text{ is bounded in } L^\infty(0, T; L^2(\Omega)),$$
$$\{\hat{u}_{h_n}^4\} \text{ is bounded in } L^\infty(0, T; L^2(\Omega)).$$

Hence, there exists a subsequence of h_n (denoted again by h_n), such that

$$\hat{u}_{h_n}^1 \rightharpoonup u^1 \text{ weakly in } L^2(S; H^1(\Omega)),$$
$$\hat{u}_{h_n}^2 \rightharpoonup u^2 \text{ weakly in } L^2(S; L^2(\Omega)),$$
$$\hat{u}_{h_n}^3 \rightharpoonup u^3 \text{ weakly in } L^2(S; L^2(\Omega)),$$
$$\hat{u}_{h_n}^4 \rightharpoonup u^4 \text{ weakly in } L^2(S; L^2(\Omega)).$$

Since

$$\|\hat{u}_{h_n}^1\|_{L^2(S, H^1(\Omega))} + \|\partial_t \hat{u}_{h_n}^1\|_{L^2(S, L^2(\Omega))} \le C,$$

Lions-Aubin's compactness theorem, see [14, Theorem 1], implies that there exists a subset (again denoted by $\hat{u}_{h_n}^1$) such that

$$\hat{u}_{h_n}^1 \longrightarrow u^1 \quad \text{strongly in} \quad L^2(S \times \Omega).$$

To get the desired strong convergence for the cell solutions $\hat{u}_{h_n}^2, \hat{u}_{h_n}^3$, we need the higher regularity with respect to the variable x, proved in Lemma 9. We remark that the two-scale regularity estimates imply that

$$\|\hat{u}_{h_n}^2\|_{L^2(S; H^1(\Omega, H^1(Y)))} + \|\hat{u}_{h_n}^3\|_{L^2(S; H^1(\Omega, H^1(Y)))} \le C.$$

Moreover, from Lemma 8, we have that

$$\|\partial_t \hat{u}_{h_n}^2\|_{L^2(S \times \Omega \times Y)} + \|\partial_t \hat{u}_{h_n}^3\|_{L^2(S \times \Omega \times Y)} \le C.$$

Since the embedding

$$H^1(\Omega, H^1(Y)) \hookrightarrow L^2(\Omega, H^\beta(Y))$$

is compact for all $\frac{1}{2} < \beta < 1$, it follows again from Lions-Aubin's compactness theorem that there exist subsequences (again denoted $\hat{u}_{h_n}^2, \hat{u}_{h_n}^3$), such that

$$(\hat{u}_{h_n}^2, \hat{u}_{h_n}^3) \longrightarrow (u^2, u^3) \quad \text{strongly in} \quad L^2(S \times L^2(\Omega, H^\beta(Y))), \tag{65}$$

for all $\frac{1}{2} < \beta < 1$. Now, (65) together with the continuity of the trace operator

$$H^\beta(Y) \hookrightarrow L^2(\partial Y), \quad \text{for} \quad \frac{1}{2} < \beta < 1,$$

yield the strong convergence of $\hat{u}_{h_n}^2, \hat{u}_{h_n}^3$ until the boundary $y = 0$. $\qquad\square$

6 Numerical illustration of the two-scale FD scheme

We close the paper with illustrating the behavior of the main chemical species driving the whole corrosion process, namely of $H_2S(g)$, and also the one of the corrosion product – the gypsum. To do these computations we use the reference parameters reported in [5].
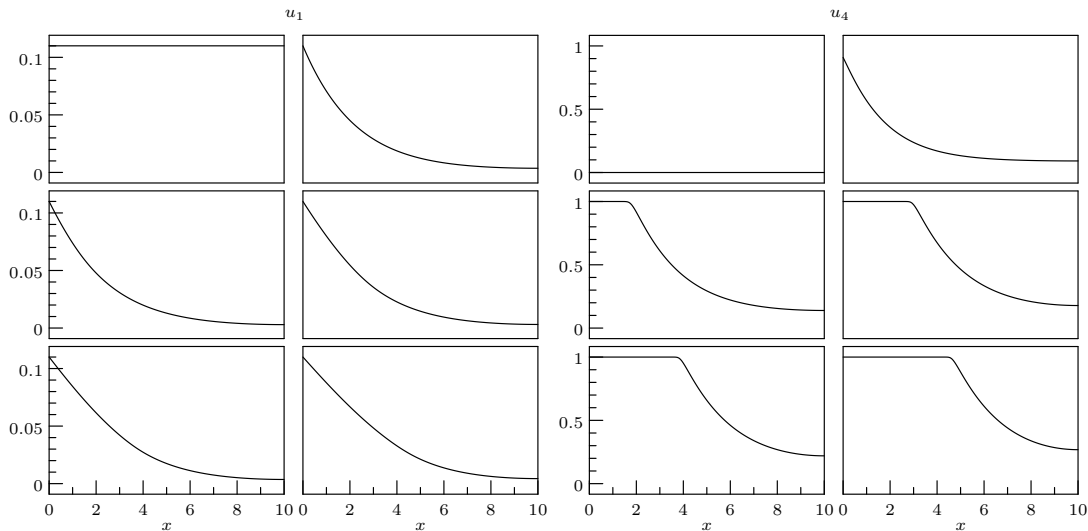

Figure 1: Illustration of concentration profiles for the macroscopic concentration of gaseous H_2S (left) and of gypsum (right). Graphs plotted at times $t \in \{0, 80, 160, 240, 320, 400\}$ in a left-to-right and top-to-bottom order.

Figure 1 shows the evolution of $u_1(x,t)$ and $u_4(x,t)$ as time elapses. Interestingly, although the behavior of u_1 is as expected (i.e., purely diffusive), we notice that a *macroscopic* gypsum layer (region where u_4 is produced) is formed (after a transient time $t^* > 80$) and grows in time. The figure clearly indicates that there are two distinct regions separated by a slowly moving intermediate layer: the left region – the place where the gypsum production reached saturation (a threshold), and the right region – the place of the ongoing sulfatation reaction (1d) (the gypsum production has not yet reached here the natural threshold). The precise position of the separating layer is *a priori unknown*. To capture it simultaneously with the computation of the concentration profile would require a moving-boundary formulation similar to the one reported in [4].

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