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# A STEFAN PROBLEM MODELLING DISSOLUTION AND PRECIPITATION IN POROUS MEDIA

T.L. VAN NOORDEN AND I.S. POP*

**Abstract.** A simple one-dimensional model for crystal dissolution and precipitation is presented. The model equations resemble a one-phase Stefan problem and involve nonlinear and multi-valued exchange rates at the free boundary. The original equations are formulated on a variable domain. By transforming the model to a fixed domain and applying a regularization, we prove the existence and uniqueness of a solution. The paper is concluded by numerical simulations.

**1. Introduction.** This work is motivated by the need for a rigorous derivation of macroscopic laws for reactive transport in porous media, and more specifically for crystal dissolution and precipitation in porous media. These laws are of practical importance in many physical, biological and chemical applications. Macroscopic laws for reactive transport in porous media are derived rigorously in, e.g., [7]. For the more specific case of crystal dissolution and precipitation, macroscopic models are given in [4, 5, 9, 12]. The analysis in these papers refers strictly to the macroscopic models and is not concerned with the rigorous derivation of the upscaled models from the micro scale ones. In most of these papers also the numerical solution of the proposed model equations is studied.

In order to give a rigorous justification of a macroscopic law, a thorough analysis and understanding of the microscale processes are needed. This is the main purpose of the work in [17]. In the cited paper, crystal dissolution and precipitation on the pore scale are studied, assuming that the crystalline layer attached to the grain surfaces is thin and does not significantly affect the geometry of the pores. The mathematical difficulties of the model in [17] are the nonlinear and multi-valued exchange rates.

In the present work we also focus on the analysis at the pore scale, however, in contrast to [17], we do take into account the change in the pore geometry due to precipitation and dissolution. We propose a one-dimensional model, which does not incorporate transport by fluid flow, but does account for the nonlinear and multi-valued exchange rates. The geometry change appears in the equations as a free boundary, comparable to the free boundary in the Stefan problem with a kinetic condition [18].

The model equations presented in this paper have much in common with model equations in other fields of applications, for example, with the Stefan type equations studied in [16] modeling an evaporation process. There the equation for the speed of the moving boundary is linear, whereas in the present work this equation is nonlinear and involves a multi-valued operator. Another field of application that benefits from analyzing and simulating dissolution and precipitation reactions is etching, see e.g., [10, 14].

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The main results presented in this paper are existence and uniqueness results for the proposed model equations. In addition we present in this paper numerical approximations to the solutions of the proposed model. The computations are performed using a finite difference method. Other methods that have been used to simulate crystal dissolution and precipitation on the pore scale are the Smoothed Particle Hydrodynamics method [15], and the Lattice Boltzmann method [8].

This paper is organized as follows. In Section 2, we introduce the model equations. We show that there exist solutions to the model equations in Section 3, and a uniqueness result is presented in Section 4. In Section 5 a numerical approximation scheme is discussed and results of the numerical experiments are shown.

**2. Model equations.** We consider the interval $[-L, L] \subset \mathbb{R}$ which is the region between two (infinite) walls, located at $x = \pm L$ [m]. Let the region $[-L, L]$ be occupied by a fluid in which cations ($M_1$) and anions ($M_2$) are dissolved. In a precipitation reaction $n_1$ cations of $M_1$, and $n_2$ anions of $M_2$ can precipitate in the form of one molecule of a crystalline solid $M_{12}$, which is attached to the boundary. The reverse dissolution reaction is also possible. We assume that precipitation leads to a homogeneous layer of crystals. The thickness of this layer is denoted by $l$ [m], and is time-dependent.

We consider here a simplified setting, where diffusion is the only transporting mechanism for the anions and cations. Let $c_i$ $[\frac{\text{mol}}{\text{m}}]$ denote the linear molar concentration of $M_i$, with $i = 1, 2$. We also assume that the whole configuration is symmetric around $x = 0$. Then $c_i$ satisfies the diffusion equation

$$\partial_t c_i = D\partial_{xx} c_i \text{ for } x \in [0, s(t)], \;\; i = 1, 2,$$

where $s(t) = L - l(t)$ is the location of the free boundary separating the fluid and the precipitate. At $x = 0$, due to symmetry, we have

$$\partial_x c_i = 0, \;\; \text{with } \; i = 1, 2.$$

Since one molecule of the precipitate contains $n_1$ cations and $n_2$ anions, conservation of mass gives

$$\int_0^{s(t)} c_1 \, dx + (L - s(t)) n_1 \rho_c = Const.,$$
$$\int_0^{s(t)} c_2 \, dx + (L - s(t)) n_2 \rho_c = Const.,$$

where $\rho_c$ $[\frac{\text{mol}}{\text{m}}]$ denotes the molar density of the crystalline solid. Differentiating with respect to $t$, we obtain:

$$s'(t) = \frac{D\partial_x c_1(s(t), t)}{n_1 \rho_c - c_1(s(t), t)} = \frac{D\partial_x c_2(s(t), t)}{n_2 \rho_c - c_2(s(t), t)}.$$

A second equation for $s(t)$ results from the description of the precipitation and dissolution process. We have

$$\rho_c l'(t) = -\rho_c s'(t) = r_p - r_d, \tag{2.1}$$

where $r_p$ $[\frac{\text{mol}}{\text{s}}]$ denotes the precipitation rate and $r_d$ $[\frac{\text{mol}}{\text{s}}]$ denotes the dissolution rate. The precipitation rate $r_p$ is expressed by

$$r_p = k_p r\big(c_1(s(t),t), c_2(s(t),t)\big), \tag{2.2}$$

where $k_p$ $[\frac{\text{mol}}{\text{s}}]$ is a positive rate constant and $r$ a rate function depending on $c_1$ and $c_2$. A typical example is given by the law of mass action kinetics, leading to

$$r(c_1, c_2) = k_m c_1^{n_1} c_2^{n_2}, \tag{2.3}$$

with $k_m$ $[\big(\frac{\text{mol}}{\text{m}}\big)^{-(n_1+n_2)}]$ a constant. For the dissolution rate $r_d$ we follow the ideas in [9] and write

$$r_d \in k_d H(l(t)) = k_d H(L - s(t)), \tag{2.4}$$

where $H$ denotes the set-valued Heaviside graph,

$$H(u) = \begin{cases} \{0\}, & \text{if} \quad u < 0, \\ [0,1], & \text{if} \quad u = 0, \\ \{1\}, & \text{if} \quad u > 0. \end{cases}$$

The relation (2.4) expresses the behavior of the dissolution rate in different cases:

1. in the presence of crystal, i.e., for $l(t) > 0$, the dissolution rate $r_d = k_d$ $[\frac{\text{mol}}{\text{s}}]$ is constant (with $k_d > 0$).
2. in the absence of crystal, i.e., $l(t) = 0$, we can identify two sub-cases:
   (a) in the undersaturated regime, i.e., $r(c_1, c_2) \le k_d/k_p$, the concentrations of $c_1$ and $c_2$ are too low to start the effective growth of a crystalline layer and the overall rate in (2.1) equals zero. In this case we have $r_p - r_d = 0$, and, using (2.2), we obtain $r_d = k_p r(c_1, c_2)$.
   (b) in the oversaturated regime, i.e., $r(c_1, c_2) > k_d/k_p$, effective growth of a crystalline layer will start with rate $r_p - k_d$, so that we set $r_d = k_d$.

The discussion above can be summarized in

$$r_d = \begin{cases} 0, & \text{if } L < s(t), \text{ or } l(t) < 0, \\ \min\{k_p r(c_1, c_2), k_d\}, & \text{if } L = s(t), \text{ or } l(t) = 0, \\ k_d, & \text{if } L > s(t), \text{ or } l(t) > 0. \end{cases} \tag{2.5}$$

If we now substitute (2.2) and (2.4) in the equation (2.1) for $s(t)$, we obtain

$$-\rho_c s'(t) \in k_d \left( \frac{k_p}{k_d} r\big(c_1(s(t),t), c_2(s(t),t)\big) - H(L - s(t)) \right). \tag{2.6}$$

From this equation, we can see that in the oversaturated regime, we have $r_p > r_d$ and precipitation ($l'(t) = -s'(t) > 0$) will occur, and that if crystal is present and we are in the undersaturated regime, dissolution ($l'(t) = -s'(t) < 0$) occurs.

**2.1. Dimensionless form.** We make the simplifying assumptions $n_1 = n_2$ and $c_1(x,0) = c_2(x,0)$, and look for solutions such that $c_1(x,t) = c_2(x,t) = c(x,t)$. We introduce reference values $t_{ref} := L^2/D$ and $x_{ref} := L$ for the time and space variables $t$ and $x$. We also introduce a reference value for the concentration $c$, denoted by $c_{ref}$. Defining

$$\begin{aligned} &t := t/t_{ref}, \quad x := x/x_{ref}, \quad v := c/c_{ref}, \quad h := s/L, \\ &\rho := \frac{n_1 \rho_c}{c_{ref}}, \quad r(v) := \frac{k_p}{k_d} r(c_{ref} v), \quad k := \frac{k_d t_{ref}}{\rho_c L}, \end{aligned}$$

gives the equations

$$\begin{cases} \partial_t v = \partial_{xx} v, & \text{for } 0 < x < h(t),\ t > 0, \\ \partial_x v = 0, & \text{for } x = 0,\ t > 0, \\ \partial_x v = (\rho - v)\partial_t h, & \text{for } x = h(t),\ t > 0, \\ \partial_t h = k(w - r(v)), & \text{for } x = h(t),\ t > 0, \\ w \in H(1-h), & \text{for } t > 0, \\ v = v_0, & \text{for } 0 \le x \le h_0,\ t = 0, \\ h = h_0, & \text{for } t = 0. \end{cases} \tag{2.7}$$

By the scaling, $h(t) \le 1$. From the model point of view, $h = 1$ means that crystals are completely dissolved so $h$ cannot exceed 1. In what follows we will prove this statement rigorously.

The dimensionless number $k$ is usually referred to as the Damköhler number and expresses the ratio between the diffusion and the reaction time scale. The auxiliary function $w$ acts as the scaled dissolution rate $r_d/k_d$. and, when $h < 1$, $w$ attains the value 1, and when $h = 1$, we have $w = r(u)$. With respect to the reaction rate function $r(v)$, we assume

1. $r : \mathbb{R} \to [0, \infty)$ is locally Lipschitz;
2. a unique $v_* \in [0, \rho)$ exists such that $r(v) = 0$ for all $v \le v_*$ and $r(v)$ is strictly increasing if $v > v_*$.
3. a unique $v^* \in (v_*, \rho)$ exists such that $r(v^*) = 1$.

Note that these assumptions are fulfilled in the typical case (2.3).

**3. Existence.** We assume that the initial data $v_0$ and $h_0$ satisfy the bounds

$$0 \le v_0(x) \le M < \rho, \text{ and } 0 < h_0 \le 1.$$

We also assume bounded initial ion concentrations and furthermore we assume that the initial data satisfy the following compatibility conditions

$$\begin{cases} v_0 \in C^2([0,h_0]), \quad \partial_x v_0(0) = 0, \\ \partial_x v_0(h_0) = k\big(r(v_0(h_0)) - w_0\big)(\rho - v_0(h_0)), \end{cases} \tag{3.1}$$

with $w_0 = w(t=0)$ defined as

$$\begin{cases} w_0 = 1, & \text{if } h_0 < 1, \\ w_0 = r(v_0(1)), & \text{if } h_0 = 1, \text{ and } v_0(1) \le v^*, \\ w_0 = 1, & \text{if } h_0 = 1, \text{ and } v_0(1) > v^*. \end{cases} \tag{3.2}$$

For a function $h \in C([0,T])$, let

$$Q_{hT} := \{(x,t) \,|\, 0 < x < h(t),\, 0 < t < T\}. \tag{3.3}$$

Definition 3.1. *We call a triple $(v,w,h)$ with*

1. $h \in C([0,T])$,
2. $v \in C^{2,1}(Q_{hT}) \cap C(\overline{Q_{hT}})$,
3. $\partial_x v \in C(Q_{hT} \cup \{x=0,\, 0 \le t \le T\})$,
4. $w \in L^\infty(0,T)$,

*a solution of (2.7) if it satisfies*

$$\begin{cases} \partial_t v = \partial_{xx} v & \text{on } Q_{hT}, \\ \partial_x v = 0 & \text{on } \{x=0,\, 0 \le t \le T\}, \\ \int_0^{h(t)} (\rho - v)\, dx = h_1, & \text{for } 0 \le t \le T, \\ h(t) = k \int_0^t \big(w(\tau) - r(v(h(\tau),\tau))\big)\, d\tau + h_0, & \text{for } 0 \le t \le T, \\ w(t) \in H(1-h(t)) & \text{a.e. in } [0,T], \\ v = v_0, & \text{for } 0 \le x \le h_0,\, t = 0, \end{cases} \tag{3.4}$$

*with $h_1 = \int_0^{h_0} (\rho - v_0(x))\, dx$.*

Note that the condition $\int_0^{h(t)} (\rho - v)\, dx = h_1$ expresses mass conservation. Because the dissolution rate $w(\tau)$ in $(2.7_4)$ may be discontinuous, $h$ may not be continuously differentiable. Therefore the boundary conditions $(2.7_{3,4})$ are not defined for every $t > 0$. To overcome this problem, in Definition 3.1, we integrate boundary condition $(2.7_4)$ in time to obtain condition $(3.4_4)$. Further,

by integrating $(2.7_1)$ in space, and using boundary conditions $(2.7_{2,3})$, we obtain $(3.4_2)$.

To prove existence of solutions of (2.7), we will take the following steps. We first apply a coordinate transform that is also used in [16] and rewrite the equation $(3.4_1)$ to a fixed domain. Then we regularize the Heaviside graph, and we prove the existence of a unique classical solution of the transformed, regularized equations. We establish, using compactness arguments, the existence of weak solutions to the transformed equations by taking the limit of the regularization parameter to zero. We show that these weak solutions are regular enough to make the inverse coordinate transform so that we obtain solutions of (2.7) in the sense of Definition 3.1. For the proof of the uniqueness result in Section 4, we use the same coordinate transform to show that uniqueness of weak solutions of the fixed domain formulation implies uniqueness of solutions in the sense of Definition 3.1.

**3.1. Coordinate transform and regularization.** We employ the coordinate transform proposed in [16]:

$$y(x,t) = \int_x^{h(t)} (\rho - v(z,t))\, dz, \quad \tau(t) = t. \tag{3.5}$$

In the new coordinates, the equations (2.7) are transformed into the following equations for the unknown concentration $u(y(x,t),\tau(t)) = v(x,t)$, which are defined on the fixed interval $[0,h_1]$

$$\begin{cases} \partial_\tau f(u) = \partial_{yy} u, & \text{for } 0 < y < h_1,\ 0 < \tau < T, \\ \partial_y u = k(r(u) - w), & \text{for } y = 0,\ 0 < \tau < T, \\ \partial_\tau h = -k(r(u) - w), & \text{for } y = 0,\ 0 < \tau < T, \\ w \in H(1-h), & \text{for } 0 < \tau < T, \\ \partial_y u = 0, & \text{for } y = h_1,\ 0 < \tau < T \\ u = u_0, & \text{for } 0 \le y \le h_1,\ \tau = 0, \\ h = h_0, & \text{for } \tau = 0, \end{cases} \tag{3.6}$$

with $f(u) = 1/(\rho - u)$, and $h_1$ as specified in Definition 3.1. For the initial condition, it holds $u_0(y(x,0)) = v_0(x)$ for $0 \le x \le h_0$. Note that the equations (3.6) are defined on the fixed interval $[0,h_1]$. Using $\partial_y u(0,\tau) = -\partial_\tau h(\tau)$ and $(3.6_1)$, we obtain the equality

$$h(t) = \int_0^{h_1} f(u) dy. \tag{3.7}$$

The next step is to regularize the Heaviside graph. With $\delta > 0$, we define

$$H_\delta(u) := \begin{cases} 0 & \text{if } v < 0, \\ u/\delta & \text{if } v \in [0,\delta], \\ 1, & \text{if } v > \delta. \end{cases}$$

Using (3.7) and replacing the Heaviside graph $H$ by $H_\delta$, gives the following problem with non-local boundary conditions

$$\begin{cases} \partial_\tau f(u) = \partial_{yy} u, & \text{for } 0 < y < h_1,\ 0 < \tau < T, \\ \partial_y u = k\left(r(u) - H_\delta\left(1 - \int_0^{h_1} f(u)dy\right)\right), & \text{for } y = 0,\ 0 < \tau < T, \\ \partial_y u = 0, & \text{for } y = h_1,\ 0 < \tau < T. \end{cases} \tag{3.8}$$

Before we state the initial data for problem (3.8), we must pay special attention to the compatibility conditions. If $h_0 < 1$, then we can choose $\delta < 1 - h_0$, and the transformed initial data $u_0$ satisfies the regularized compatibility condition

$$\partial_y u_0(0) = k\left(r(u_0(0)) - H_\delta\left(1 - \int_0^{h_1} f(u_0(y))dy\right)\right). \tag{3.9}$$

Also if $h_0 = 1$ and $u_0(0) \le v_*$ so that $r(u_0(0)) = 0$, the initial data $u_0$ satisfies the regularized compatibility condition (3.9). If $h_0 = 1$ and $u_0(0) > v_*$ then the initial data $u_0$ does not satisfy (3.9). To resolve this problem, we modify the initial data depending on $\delta$, and such that the condition in (3.9) is satisfied. We define $u_{0,\delta}$ in the following way

$$u_{0,\delta} := \begin{cases} u_0 & \text{if } h_0 < 1 \text{ or } u_0(0) \le v_*, \\ C_\delta u_0 & \text{if } h_0 = 1 \text{ and } v_* < u_0(0) \le v^*, \\ c_\delta u_0 & \text{if } h_0 = 1 \text{ and } u_0(0) > v^*, \end{cases} \tag{3.10}$$

with $C_\delta$ and $c_\delta$ such that

$$\begin{aligned} 1 - \int_0^{h_1} f(C_\delta u_0)dy &= \delta\, r\big(C_\delta u_0(0)\big), \\ 1 - \int_0^{h_1} f(c_\delta u_0)dy &= \delta\, r\big(c_\delta u_0(0)\big) - \delta\, c_\delta\big(r\big(u_0(0)\big) - 1\big). \end{aligned}$$

In Appendix A it is shown that such $c_\delta$ and $C_\delta$ exist and that $0 \le c_\delta \le 1$ and $0 \le C_\delta \le 1$. Furthermore, as $\delta \searrow 0$ we have $c_\delta \nearrow 1$ and $C_\delta \nearrow 1$, so that $u_{0,\delta} \to u_0$ for $\delta \to 0$. We see that $u_{0,\delta}$ satisfies the compatibility conditions

$$\begin{cases} u_{0,\delta} \in C^2([0, h_1]), \quad \partial_y u_{0,\delta}(h_1) = 0, \\ \partial_y u_{0,\delta}(0) = k\left(r(u_{0,\delta}(0)) - H_\delta\left(1 - \int_0^{h_1} f(u_{0,\delta}(y))dy\right)\right), \end{cases} \tag{3.11}$$

and also

$$0 \le u_{0,\delta}(y) \le u_0(y) \le M < \rho. \tag{3.12}$$

Now we supplement the equations (3.8) with the intial condition

$$u = u_{0,\delta} \text{ for } 0 \le y \le h_1,\ \tau = 0. \tag{3.13}$$

The equations (3.8) and (3.13) are closely related to the equations studied in [1], and the iteration procedure discussed below is based on arguments in [1]. A classical solution of the equations (3.8) and (3.13) is defined in the usual sense: let

$$Q_T := (0, h_1) \times (0, T),$$

then a classical solution $u$ satisfies (3.8) and (3.13) with

1. $u \in C^{2,1}(Q_T) \cap C(\overline{Q_T})$,
2. $u_y \in C(\overline{Q_T})$.

We first start with a boundedness result.

LEMMA 3.2. *Let $u$ be a classical solution of* (3.8) *with initial conditions (3.12-3.13), then* $0 \le u(y,\tau) \le \max(M, v^*)$.

*Proof.* Let $M_0 = \max(M, v^*)$. We use ideas from [2]: for small $\epsilon > 0$ we define $\psi_\epsilon(z) := H_\epsilon(z)$ and we write

$$\int_0^{h_1} \partial_\tau (f(u) - f(M_0))\psi_\epsilon(u - M_0)dy = \int_0^{h_1} \partial_{yy}(u - M_0)\psi_\epsilon(u - M_0)dy.$$

To avoid confusion with the regularized dissolution rate, we have used the notation $\psi_\epsilon$. Integration by parts gives

$$\int_0^{h_1} \partial_\tau (f(u) - f(M_0))\psi_\epsilon(u - M_0)dy + \int_0^{h_1} (\partial_y(u - M_0))^2 \psi'_\epsilon(u - M_0)dy \\ = -k\big(r(u) - H_\delta(1 - h)\big)\psi_\epsilon(u - M_0)|_{y=0}.$$

Taking the limit $\epsilon \to 0$, which is allowed since $\int_0^{h_1} |\partial_\tau (f(u) - f(M_0))|dy$ is bounded, see [11, Lemma V.7.2], and using that $\psi'_\epsilon \ge 0$ and that for $u > M_0$ we have $r(u) > 1$, we obtain

$$\partial_\tau \int_0^{h_1} [f(u) - f(M_0)]_+ dy \le 0,$$

so that we may conclude $u \le M_0$. A similar reasoning proves $0 \le u$. □

Now we introduce the mapping $F$ by the following procedure: given a function $u_{i-1} \in C^{2,1}(\overline{Q_T})$, we define the function $u_i$ by solving

$$\begin{cases} \partial_\tau f(u_i) = \partial_{yy} u_i, & \text{for } 0 < y < h_1,\ 0 < \tau < T, \\ \partial_y u_i = k\big(r(u_i) - H_\delta(1 - h^{(i-1)})\big), & \text{for } y = 0,\ 0 < \tau < T, \\ \partial_y u_i = 0, & \text{for } y = h_1,\ 0 < \tau < T, \\ u = u_{0,\delta}, & \text{for } 0 \le y \le h_1,\ \tau = 0, \end{cases} \tag{3.14}$$

where $h^{(i-1)}(\tau) = \int_0^{h_1} f(u_{i-1})dy$. Given a differentiable $h(\tau)$, (3.14) has a unique classical solution in $C^{2,1}(\overline{Q_T})$, see [11, Theorem V.7.4]. In this way the operator $F$ is defined as an operator from $C^{2,1}(\overline{Q_T})$ into itself. Furthermore, again by [11, Lemma V.7.2] and by using Lemma 3.2 and the continuous differentiability of $f$, the integrals $\int_0^{h_1} |\partial_\tau f(u_i)|dy$ are bounded.

LEMMA 3.3. *For $\tilde{T} < \delta$, the mapping $F$ is a contraction with respect to the $C([0,\tilde{T}]; L^1(0,h_1))$ norm.*

*Proof.* Consider two solutions $u_{i-1}$ and $\tilde{u}_{i-1}$, both in $C^{2,1}(\overline{Q_T})$, and define $u_i := F(u_{i-1})$ and $\tilde{u}_i := F(\tilde{u}_{i-1})$, obtained by solving (3.14) with $h^{(i-1)} = \int_0^{h_1} f(u_{i-1})dy$ and $\tilde{h}^{(i-1)} = \int_0^{h_1} f(\tilde{u}_{i-1})dy$ respectively. Now we proceed similarly as in the proof of Lemma 3.2: we subtract the equations (3.14) for $u_i$ and $\tilde{u}_i$ and test the result with a regularized sign-function. Specifically, we consider a smooth convex function $m : \mathbb{R} \to \mathbb{R}$ with

$$m \geq 0, \quad m(0) = 0, \quad m(r) = |r| - \frac{1}{2} \text{ for } |r| > 1,$$

and define for $\epsilon > 0$ approximations of the modulus function by

$$m_\epsilon := \epsilon m\left(\frac{r}{\epsilon}\right).$$

We test the equations for $u_i - \tilde{u}_i$ with $\chi_{[0,t]} m_\epsilon'(u_i - \tilde{u}_i)$, where $t \leq \tilde{T}$ is arbitrary, and obtain, after sending $\epsilon$ to zero,

$$\begin{aligned}
&\int_0^{h_1} |f(u_i) - f(\tilde{u}_i)|dy \\
&\leq \int_0^t \left( H_\delta\left(1 - \int_0^{h_1} f(u_{i-1})dy\right) - H_\delta\left(1 - \int_0^{h_1} f(\tilde{u}_{i-1})dy\right)\right) \operatorname{sgn}(u_i - \tilde{u}_i)|_{y=0} d\tau \\
&\quad -k \int_0^t \big(r(u_i) - r(\tilde{u}_i)\big) \operatorname{sgn}(u_i - \tilde{u}_i)|_{y=0} d\tau.
\end{aligned}$$

Since $r$ is increasing, and using the Lipschitz continuity of $H_\delta$, we can majorize the right-hand side above by

$$\sup_{\tau \in [0,\tilde{T}]} \frac{\tilde{T}}{\delta} \int_0^{h_1} |f(u_{i-1}) - f(\tilde{u}_{i-1})|dy$$

This estimate is uniform in $t$, therefore it holds that

$$\sup_{\tau \in [0,\tilde{T}]} \int_0^{h_1} |f(u_i) - f(\tilde{u}_i)|dy \leq \sup_{\tau \in [0,\tilde{T}]} \frac{\tilde{T}}{\delta} \int_0^{h_1} |f(u_{i-1}) - f(\tilde{u}_{i-1})|dy$$

Because $\tilde{T} < \delta$, the operator $F$ is a contraction on $C^{2,1}(\overline{Q_{\tilde{T}}})$ in the norm of the Banach space $C([0,\tilde{T}];L^1(0,h_1))$. □

REMARK 3.4. Using the density of $C^{2,1}(\overline{Q_{\tilde{T}}})$ in $C([0,\tilde{T}];L^1(0,h_1))$ and Lemma 3.3, we can extend the operator $F$ to a contraction from $C([0,\tilde{T}];L^1(0,h_1))$ into itself.

LEMMA 3.5. *Let the sequence $\{u_i\}$ be defined by $u_i = F(u_{i-1})$ with a given $u_0$. Then $\{u_i(0,t)\}$ is a Cauchy sequence in $C([0,\tilde{T}])$.*

*Proof.* Let $\epsilon > 0$ be given. Since $F$ is a contraction, $\{u_i\}$ is a Cauchy sequence in $C([0,T];L^1(0,h_1))$. By [11, Theorem V.7.2], the sequence $\{\partial_y u_i\}$ is bounded in $L^\infty(Q_T)$. This implies the existence of a $\mu > 0$ such that $\int_0^\mu |\partial_y(u_m - u_n)|dy < \epsilon/3$ for all $m,n \in \mathbb{N}$. Because $\{u_i\}$ is a Cauchy sequence in $C([0,\tilde{T}];L^1(0,h_1))$, with $\tilde{T} < \delta$, there is a $N_0$ such that $\sup_\tau \int_0^{h_1} |u_m(y,\tau) - u_n(y,\tau)|dy < \mu\epsilon/3$ for all $m,n > N_0$. It follows that

$$\sup_{\tau\in[0,\tilde{T}]} |u_m(0,\tau) - u_n(0,\tau)|$$
$$\leq \sup_{\tau\in[0,\tilde{T}]} \left(\frac{1}{\mu}\int_0^\mu |u_m(y,\tau) - u_n(y,\tau)|dy + \int_0^\mu |\partial_y(u_m - u_n)|dy\right) < \epsilon,$$

for all $m,n > N_0$. □

THEOREM 3.6. *Assuming* (3.11) *and* (3.12)*, there exists a unique classical solution $u_\delta$ of* (3.8) *with initial condition* (3.13).

*Proof.* Lemma 3.3 provides the existence of a unique fixed point $u_\delta \in C([0,\tilde{T}];L^1(0,h_1))$, with $\tilde{T} < \delta$, of $F$. In order to show that this fixed point is indeed a classical solution of (3.8), we need to show higher regularity of $u_\delta$.

Let $\{u_i\}$ be a sequence in $C^{2,1}(\overline{Q_{\tilde{T}}})$ generated by iterating $F$, converging to $u_\delta$ in $C([0,\tilde{T}];L^1(0,h_1))$. We have

$$\int_0^{h_1} f(u_i(y,t))dy = h_{0,\delta} - k\int_0^t \left(r(u_i) - H_\delta\left(1 - \int_0^{h_1} f(u_{i-1})dy\right)\right)d\tau,$$

where $h_{0,\delta} := \int_0^{h_1} f(u_{0,\delta})dy$. By Lemma 3.5, $u_i(0,\tau)$ converges uniformly to $u_\delta(0,\tau)$. Since $f$, $r$ and $H_\delta$ are continuous, we conclude that $\int_0^{h_1} f(u_\delta)dy$ is a $C^1$ function in time. Taking this into account in $(3.14_2)$, it follows that the boundary data for $y = 0$ are in $C^1([0,\tilde{T}])$. Therefore, by [11, Theorem V.7.4], $u_\delta$ is a classical solutions of (3.8) with initial condition (3.13).

To extend the time interval of existence, we note that Lemma 3.2 guarantees that the solution $u_\delta$ remains bounded. Therefore we can restart the iteration at, say, $t = \delta/2$. It follows that the solution exists on the entire interval $(0,T]$. □

We now proceed by obtaining an estimate that is uniform in $\delta$.

LEMMA 3.7. *For $\delta > 0$, the classical solution $u_\delta$ of (3.8) satisfies*

$$\int_0^{h_1} |u_\delta(y,t)|^2\,dy + \int_0^t\int_0^{h_1} |\partial_y u_\delta|^2\,dyd\tau + \|\partial_\tau f(u_\delta)\|_{L^2(0,t;H^{-1}(0,h_1))} \le K,$$

*for $0 < t < T$, where $K > 0$ does not depend on $\delta$.*

*Proof.* The first term $\int_0^{h_1} |u_\delta(y,t)|^2\,dy$ is bounded uniformly in $\delta$ by Lemma 3.2. For the second term, we fix an arbitrary $t \in (0,T]$, multiply $(3.8_1)$ with $u_\delta$ and integrate in both time and space to obtain

$$\int_0^t\int_0^{h_1} \partial_\tau f(u_\delta)u_\delta\,dyd\tau = \int_0^t\int_0^{h_1} (\partial_{yy}u_\delta)u_\delta\,dyd\tau.$$

Using the definition of $f(u_\delta)$, and integrating by parts, we obtain

$$\begin{aligned}\int_0^{h_1} \frac{\rho}{\rho-u_\delta} + \ln|\rho-u_\delta|\,dy + \int_0^t\int_0^{h_1} |\partial_y u_\delta|^2\,dyd\tau \\ = -k\int_0^t \left(r(u_\delta) - H_\delta\left(1 - \int_0^{h_0} f(u_\delta)dy\right)\right)\,dt.\end{aligned}$$

Since $u_\delta$ is bounded, this immediately yields the uniform bound on $\int_0^t\int_0^{h_1} |\partial_y u_\delta|^2\,dyd\tau$.

For the last part of the lemma, we notice that

$$\begin{aligned}\int_0^{h_1} \partial_\tau f(u_\delta)\phi\,dy = -k\left(r(u_\delta(0,t) - H_\delta\left(1 - \int_0^{h_0} f(u_\delta)\,dy\right)\right)\phi(0) \\ - \int_0^{h_1} \partial_y u_\delta \partial_y \phi\,dy,\end{aligned}$$

for all $\phi \in H^1(0,h_1)$. The $L^\infty$ estimates on $u_\delta$, together with the trace theorem for $\phi$, gives

$$\left|\int_0^{h_1} \partial_\tau f(u_\delta)\phi\,dy\right| \le \left(kC\big(r(M_0)+1\big) + \int_0^{h_1} |\partial_y u_\delta|^2\,dy\right)\|\phi\|_{H^1(0,h^1)}.$$

Since $\phi \in H^1(0,h_1)$ is arbitrary, we can use the estimate on $\int_0^t\int_0^{h_1} |\partial_y u_\delta|^2\,dyd\tau$, to conclude the remaining part of the lemma. ∎

**3.2. The limit $\delta \searrow 0$.** By sending $\delta$ to zero, a classical solution of (3.6) cannot be expected. This is because $u_y(0,\tau)$ may have jumps whenever $h$ arrives in or leaves the boundary $y = h_1$. Therefore we need a weak formulation of the problem. Let

$$\begin{aligned}U &:= \{u \in L^2(0,T;H^1(0,h_1)) \ : \ \partial_t u \in L^2(0,T;H^{-1}(0,h_1))\},\\ V &:= \{w \in L^\infty(0,T),\ 0 \le w \le 1\},\\ W &:= C([0,T]),\end{aligned}$$

and let $(\cdot,\cdot)$ denote the inner product in $L^2(0,h_1)$. Further, by $<\cdot,\cdot>$ we mean the duality pairing between $H^{-1}(0,h_1)$ and $H^1(0,h_1)$.

DEFINITION 3.8. *A triple $(u,w,h) \in U \times V \times W$ is called a weak solution of (3.6) if*

$$\begin{aligned} \int_0^T <\partial_\tau f(u),\phi> d\tau + \int_0^T (\partial_y u, \partial_y \phi) d\tau \\ +k\int_0^T \big(r(u(0,\tau)) - w(\tau)\big)\phi(0,\tau) d\tau = 0, \end{aligned} \tag{3.15}$$

*for all $\phi \in L^2(0,T;H^1(0,h_1))$ and if in addition*

$$w \in H(1-h) \quad a.e.\ in\ [0,T], \tag{3.16}$$

$$h(\tau) = h_0 - k\int_0^\tau \big(r(u(0,t)) - w(t)\big) dt, \tag{3.17}$$

$$u(y,0) = u_0(y) \quad for \quad 0 < y < h_1. \tag{3.18}$$

Lemma 3.7 gives the necessary uniform estimates to establish the existence of a triple $(u,w,h) \in U \times V \times W$ and of a sequence $\delta \searrow 0$, such that

1. $u_\delta \to u$ weakly in $L^2(0,T;H^1(0,h_1))$,
2. $\partial_\tau f(u_\delta) \to g$ weakly in $L^2(0,T;H^{-1}(0,h_1))$.

Further, since $H_\delta\left(1 - \int_0^{h_1} f(u_\delta)\, dy\right) \in L^\infty(0,T)$, we have

3 $w_\delta := H_\delta\left(1 - \int_0^{h_1} f(u_\delta)\, dy\right) \to w$ weakly-star in $L^\infty(0,T)$,

and finally, by the Arzela-Ascoli theorem,

4 $h_\delta := h_{0,\delta} - k\int_0^\tau \big(r(u_\delta(0,t)) - w_\delta(t)\big) dt \to h$ in $C([0,T])$.

THEOREM 3.9. *The triple $(u,w,h)$ is a weak solution of (3.6).*

*Proof.* First, we observe that the sequence $\{u_\delta\}$, for $\delta \searrow 0$, is bounded in $L^2(0,T;H^1(0,h_1))$ and that $f(u)$ is a $C^1$ function of $u$ for $0 \le u \le M$. By the chain rule, see [6, Theorem 7.7.8], the sequence $\{f(u_\delta)\}$ is bounded in $L^2(0,T;H^1(0,h_1))$. Because $\{\partial_\tau f(u_\delta)\}$ is a bounded sequence in $L^2(0,T;H^{-1}(0,h_1))$, it follows that the sequence $\{f(u_\delta)\}$ is a bounded sequence in $C([0,T];L^2(0,h_1))$, see [13, Lemma 9, Corollary 4]. This gives the existence of a $\tilde{g}$ such that

$$\{f(u_\delta)\} \to \tilde{g} \ \text{ strongly in } \ L^2(0,T;H^s[0,h_1]),$$

for any $s < 1$. Since $f^{-1}$ is continuously differentiable and $\{f(u_\delta)\}$ converges a.e. to $\tilde{g}$, the sequence $\{u_\delta\}$ converges a.e. to $f^{-1}(\tilde{g})$. Because $\{u_\delta\}$ converges weakly to $u$, it follows that $f(\tilde{g}) = u$, or $\tilde{g} = f^{-1}(u)$ a.e. Now, since $\{\partial_\tau f(u_\delta)\}$ converges to $g$ and $\{f(u_\delta)\}$ converges to $f(u)$, it follows that $g = \partial_\tau f(u)$.

The trace theorem and the convergence of $\{u_\delta\}$ in $L^2(0,T;H^s(0,h_1))$ for $s<\frac{1}{2}$, implies the strong convergence of $\{u_\delta(0,t)\}$ to $u(0,t)$ in $L^2(0,T)$.

The weak convergence of $u_\delta$ and of $\partial_\tau f(u_\delta)$, the weak-star convergence of $w_\delta$ and the convergence of $\{u_\delta(0,t)\}$ imply that $u$ and $w$ satisfy (3.15). By the strong convergence of $\{u_\delta(0,t)\}$ and the weak-star convergence of $w_\delta$, we see that (3.17) holds and by construction of the compatibility conditions (3.11), we see that the equation (3.18) is satisfied.

It remains to be shown that (3.16) holds. We decompose the interval $[0,T]$ into $S_1$ and $S_2$, where

$$S_1=\{t\in[0,T]|h(t)<1\}\quad\text{and}\quad S_2=\{t\in[0,T]|h(t)=1\}.$$

We consider two cases:

1. $t\in S_1$: there exists a $\mu>0$ such that $h(t)<1-2\mu$. There also exists a $\delta_\mu>0$ such that $h_\delta(t)<1-\mu$ for all $\delta<\delta_\mu$. This means that $1-\int_0^{h_1}f(u_\delta)dy>\mu$, and thus $w_\delta(t)=1$ for all $\delta<\min(\delta_\mu,\mu)$. This implies $w(t)=1$ for $t\in S_1$.

2. $t\in S_2$: in this case $h=1$ and $h'(t)=0$ a.e in $S_2$. Differentiating (3.17), we obtain that $h'(t)=k(w(t)-r(u(0,t)))$ a.e. in $S_2$. It follows that $w(t)=r(u(0,t))$ a.e. in $S_2$, with $r(u(0,t))\leq 1$.

Summarizing, we see that $w\in H(1-h)$ a.e. in $[0,T]$. This concludes the proof. □

REMARK 3.10. As follows from the proof, we have that $w(t)=r(u(0,t))$ for almost every $t\in[0,T]$ with $h(t)=1$.

We now turn our attention to the model (2.7) in the original, variabel domain formulation. To this aim we first proof that $\partial_y u$ is essentially bounded in $Q_T$.

LEMMA 3.11. *Given a weak solution $(u,w,h)$ of (3.6), a $K>0$ exists such that*

$$|\partial_y u|\leq K\ \ \textit{a.e. in}\ Q_T.$$

*Proof.* We consider the following problem for $v=\partial_y u$

$$\begin{cases}\partial_\tau v=\partial_y(\frac{1}{f'(u)}\partial_y v), & \text{for } 0<y<h_1,\ 0<\tau<T,\\ v=k(r(u)-w), & \text{for } y=0,\ 0<\tau<T,\\ v=0, & \text{for } y=h_1,\ 0<\tau<T,\\ v=\partial_y u_0, & \text{for } 0\leq y\leq h_1,\ \tau=0,\end{cases}$$

which is obtained by differentiating (3.6) with respect to $y$. These equations have a unique weak solution $v\in L^2(0,T;H^1(0,h_1))$ with $\partial_\tau v\in L^2(0,T;H^{-1}(0,h_1))$,

see e.g., Theorem 3, Chapter 7 in [3]. We test with $[v-K_1]_+$, where $K_1 = \max\Big(\text{ess sup}_{0\le\tau\le T} k\big(r(u(0,\tau))-w(\tau)\big), \sup_{0\le y\le h_1}(\partial_y u_0), 0\Big)$, and obtain

$$\int_0^T < \partial_\tau v, [v-K_1]_+ > d\tau + \int_0^T \left(\frac{1}{f'(u)}\partial_y v,\ \partial_y([v-K_1]_+)\right) d\tau$$
$$= \int_0^T \frac{1}{f'(u)}\partial_y v[v-K_1]_+|_{y=0}^{y=h_1} d\tau.$$

Since $v = f(r(u)-w) \le K$ at $y=0$, it follows that

$$\int_0^{h_1} \frac{1}{2}([v-K_1]_+)^2 dy + \int_0^T\int_0^{h_1} \frac{1}{f'(u)}\big(\partial_y[v-K_1]_+\big)^2 dy d\tau = 0.$$

Therefore $v \le K_1$ a.e. in $Q_T$. Similarly we can show that $v \ge K_2$ a.e. in $Q_T$ with $K_2 = \min\Big(\text{ess inf}_{0\le\tau\le T} k\big(r(u(0,\tau))-w(\tau)\big), \inf_{0\le y\le h_1}(\partial_y u_0), 0\Big)$, and the result follows, with $K = \max(K_1, K_2)$. □

THEOREM 3.12. *There exists a solution of* (2.7) *in the sense of Definition 3.1.*

*Proof.* By [11, Theorem III.10.1] a weak solution of (3.6) obtained by Theorem 3.9, is actually in $C^{2,1}(\overline{Q_T}\backslash\{y=0,\ 0<\tau<T\})$ and satisfies the equations $\partial_\tau f(u) = \partial_{yy} u$ in $Q_T$ and $\partial_y u = 0$ in $\{y=h_1,\ 0<\tau<T\}$, and also the initial conditions. To establish the membership of $u$ in $C(\overline{Q_T})$, we write

$$u(0,\tau) = u(h_1,\tau) - \int_0^{h_1} \partial_y u(y,\tau)\, dy.$$

We know that $u(h_1,\tau)$ is continuous in $\tau$. Furthermore we know that $\partial_y u(y,\tau)$ is continous in $\tau$ for $0 < y < h_1$ and that $\max_{\overline{Q_T}}|\partial_y u| < K$, by Lemma 3.11. It follows by the dominated convergence theorem that $\int_0^{h_1}\partial_y u(y,\tau)\,dy$ is continuous in $\tau$, and thus the same holds for $u(0,\tau)$. Therefore $u \in C(\overline{Q_T})$.

Using the coordinate transform

$$x = \int_y^{h_1} f(u) d\bar{y}, \quad t(\tau) = \tau, \tag{3.19}$$

which is the inverse transform of (3.5), we obtain a function $v(x(y),t(\tau)) = u(y,\tau)$ that is in $C^{2,1}(Q_{hT}) \cup C(\overline{Q_{hT}})$ and satisfies the equation $\partial_t v = \partial_{xx} v$ on $Q_{hT}$ and $\partial_x v = 0$ on $\{x=0,\ 0\le t\le T\}$.

By substituting $u(0,t) = v(h(t),t)$ in the equality $h(t) = k\int_0^t (w(\tau) - u(0,\tau))d\tau + h_0$, we get the desired equation for $h(t)$ in Definition 3.1. By the coordinate transform, we have

$$h_1 = \int_0^{h_1} dy = \int_0^{h(t)} (\rho - v)\, dx.$$

This shows that all the requirements in Definition 3.1 are fulfilled and the result follows. □

REMARK 3.13. Using similar arguments as in the proof of Lemma 3.2, we can show that for weak solutions $u$ of (3.6) the result in Lemma 3.2 also holds, i.e., $0 \le u(y,\tau) \le \max(M, v^*)$. This result remains of course valid for the solution $v(x,t)$ of (2.7) obtained from $u$ by the transform (3.19), so that we also have

$$0 \le v(x,t) \le \max(M, v^*).$$

Using the lower bound for $v$ and $(3.4_3)$, we bound $h(t)$ from below, and using the continuity of $h$ and the fact that $\partial_t h \le 0$ for $h > 1$, we bound $h(t)$ from above, giving

$$\frac{h_1}{\rho} \le h(t) \le 1.$$

**4. Uniqueness.** In this section we prove that (2.7) has a unique solution.

THEOREM 4.1. *There exists at most one solution of* (2.7) *in the sense of Definition 3.1.*

*Proof.* Suppose we have two solution $(v,w,h)$ and $(\tilde v, \tilde w, \tilde h)$ to the equations (2.7). Using the coordinate transform (3.5), we transform these solution into weak solutions $(u,w,h)$ and $(\tilde u, \tilde w, \tilde h)$ of (3.6). From the Theorems 2.3 and 2.4 in [2], it follows that both $\partial_\tau f(u)$ and $\partial_\tau f(\tilde u)$ are in $L^2(Q_T)$. Now we proceed again as in the proof of Lemma 3.2 and define again $\psi_\epsilon(z) := H_\epsilon(z)$. With $t \in (0,T]$ fixed arbitrarily, we test the equations for $u$ and $\tilde u$ with $\chi_{[0,t]}\psi_\epsilon(u-\tilde u)$ and the equations for $h$ and $\tilde h$ with $\chi_{[0,t]}\psi_\epsilon(\tilde h - h)$, and sum to obtain

$$\begin{aligned}
&\int_0^t < \partial_\tau(f(u) - f(\tilde u)), \psi_\epsilon(u-\tilde u) > d\tau \\
&\quad + \int_0^t\int_0^{h_1} (\partial_y(u-\tilde u))^2 \psi_\epsilon'(u-\tilde u) dy d\tau + \int_0^t \partial_\tau(\tilde h - h)\psi_\epsilon(\tilde h - h) d\tau \\
&\quad + k\int_0^t \big(r(u) - r(\tilde u) - H(1-h) + H(1-\tilde h)\big)\big(\psi_\epsilon(u-\tilde u) - \psi_\epsilon(\tilde h - h)\big) d\tau = 0.
\end{aligned}$$

Since $\psi_\epsilon' \ge 0$, letting $\epsilon \searrow 0$ gives the estimate

$$\begin{aligned}
&\left(\int_0^{h_1} [f(u) - f(\tilde u)]_+ dx + [\tilde h - h]_+\right)\Bigg|_{\tau=t} \\
&\qquad \le -k\int_0^t \big(r(u) - r(\tilde u) - H(1-h) + H(1-\tilde h)\big)\big(H(u-\tilde u) - H(\tilde h - h)\big) d\tau.
\end{aligned}$$

By the monotonicity of $H$ and of $r$, the expression on the right is nonpositive. Since $t \in (0,T]$ was chosen arbitrarily, we obtain that $u(y,t) \le \tilde u(y,t)$ for all

$(y,\tau) \in Q_T$ and $\tilde{h}(\tau) \leq h(\tau)$ for all $0 < \tau < T$. By reversing the roles of $(u,w,h)$ and $(\tilde{u},\tilde{w},\tilde{h})$ we obtain the opposite inequalities, and thus $(u,w,h) = (\tilde{u},\tilde{w},\tilde{h})$. Hence also $(v,w,h) = (\tilde{v},\tilde{w},\tilde{h})$. □

REMARK 4.2. In Section 3.2, we obtained the existence of a subsequence $\delta \searrow 0$, such that $\{u_\delta\}$ converges to $u$ along this subsequence. As a corollary to Theorem 4.1 we can now assert that $\{u_\delta\}$ converges to $u$ along any sequence $\delta \searrow 0$.

**5. Numerical examples.** In this section we present numerical examples for the dimensionless model (2.7). First we approximate the solution of the regularized and transformed equations (3.8) using the implicit Euler scheme, and then we make the inverse transform to plot the solutions in the original, variable, coordinates.

The dimensionless parameters and data used for the first example are

$$\rho = 1, \quad h_0 = 0.5, \quad v_0 \equiv 0, \quad k = 1,$$

and the nonlinear reaction rate is given by $r(v) = 3v^2$. The region between $y = h_0 = 0.5$ and $y = L = 1$ is occupied by precipitate and since $v_0 < v^*$ only dissolution can be encountered. For the transformed equations (3.8), this gives the parameters and data

$$h_1 = 0.5, \quad u_0 \equiv 0.$$

Note that the nonlinear rate function gives the value $u^* = 1/\sqrt{3} \approx 0.577$. As in the existence proof, the computations are performed for a regularized model with $\delta = 0.01$.

For the discretization of equations (3.8), we first fix a time step $\Delta\tau > 0$ and a number $n+1 \in \mathbb{N}$ of equidistant spatial nodes. This divides the interval $[0, h_1]$ into $n$ sub-intervals of length $\Delta y = \frac{h_1}{n}$. For $j = 1, ..., n$ and $m = 0, 1, 2, ...$, we introduce the approximations $u_j^m \approx u(y_j, \tau_m)$, where $y_j = j\Delta y$ and $\tau_m = m\Delta\tau$. These approximations are obtained by solving

$$\begin{aligned}
&\frac{f(u_j^{m+1}) - f(u_j^m)}{\Delta\tau} = \frac{u_{j-1}^{m+1} - 2u_j^{m+1} + u_{j+1}^{m+1}}{(\Delta y)^2}, \quad \text{for} \quad j = 2, ..., n, \\
&\frac{f(u_0^{m+1}) - f(u_0^m)}{\Delta\tau} = \frac{2u_1^{m+1} - 2u_0^{m+1}}{(\Delta y)^2} - \frac{2k}{\Delta y}\Bigg( r(u_0^{m+1}) \\
&\qquad\qquad - H_\delta\Big(1 - \frac{1}{2\Delta y}\sum_{j=0}^{n}[f(u_j^{m+1}) + f(u_{j+1}^{m+1})]\Big)\Bigg), \\
&\frac{f(u_{n+1}^{m+1}) - f(u_{n+1}^m)}{\Delta\tau} = \frac{2u_n^{m+1} - 2u_{n+1}^{m+1}}{(\Delta y)^2},
\end{aligned}$$

for $m = 0, 1, 2, ...$ Note that the last two equations incorporate the boundary conditions, and that the integral in (3.8) is replaced by the repeated trapezoidal rule. This results in a system of nonlinear equations that we solve using Newton's method.

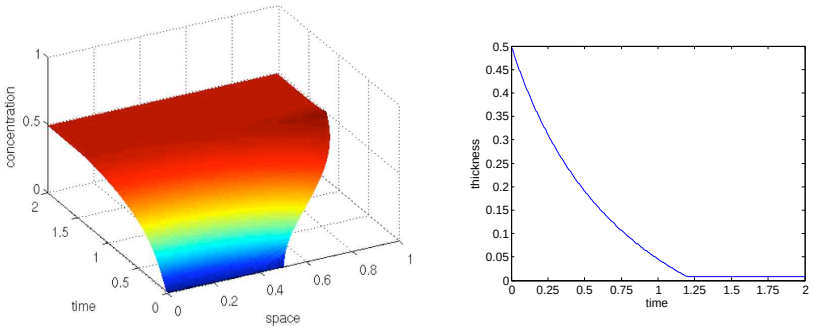


FIG. 5.1. *Results for the first experiment, left plot: the evolution of the concentration $v$ in time displayed in the original coordinates; right plot: the thickness of the crystal layer $h(t)$ versus time.*

For the first numerical experiment we divide the interval $[0, h_1] = [0, 0.5]$ in $n = 100$ subintervals so that we obtain 101 equidistant nodes with $\Delta y = 0.005$. For $\Delta\tau$ we take 0.005.

For plotting the solution $v(x,t) = u(y(x,t), \tau(t))$ in the original coordinates $x$ and $t$, we perform the inverse coordinate transform of (3.5), given by (3.19). The approximate solution $v$ is presented in Figure 5.1 using the original, variable, coordinates. In the same figure, on the right, the thickness of the crystal layer $h(t) = \int_0^{h_1} f(u)dy$ is depicted.

We see that the thickness of the crystal layer is decreasing in time. Consequently the ion concentration in the fluid is increasing. Around $t = 1.25$ the entire precipitate is dissolved, and the ion concentration is approaching the steady state $v \equiv 0.5$. Because $0.5 < u^* \approx 0.577$, there are no crystals present in the steady state. We see that the total mass is conserved, since also initially the total mass of the ions was equal to 0.5.

For the second numerical experiment we use the parameters

$$\rho = 1, \quad h_0 = 0.95, \quad k = 20,$$

and the nonlinear reaction rate is again given by $r(v) = 3v^2$. The initial ion concentration is a step function with maximal value $v = 0.8$ and minimal value $v = 0$ and with the jump at $x = 19/24 \approx 0.79$. This value is chosen such that the the jump of the step function in the transformed coordinates is located at $y = h_1/2$. For the transformed equations (3.8), this gives the parameter value $h_1 = 19/60$. Furthermore we use for the regularized Heaviside graph the value $\delta = 0.003$. We divide again the interval $[0, h_1] = [0, 0.5]$ in $n = 100$ subintervals so that we obtain 101 equidistant nodes with $\Delta y = h_1/100 \approx 0.0079$. For $\Delta\tau$ we take 0.000125.

In Figure 5.2 we present in the left plot the concentration $v$ against $t$ and $x$ and in the right plot the thickness of the crystal layer $h(t)$ against $t$. We see that

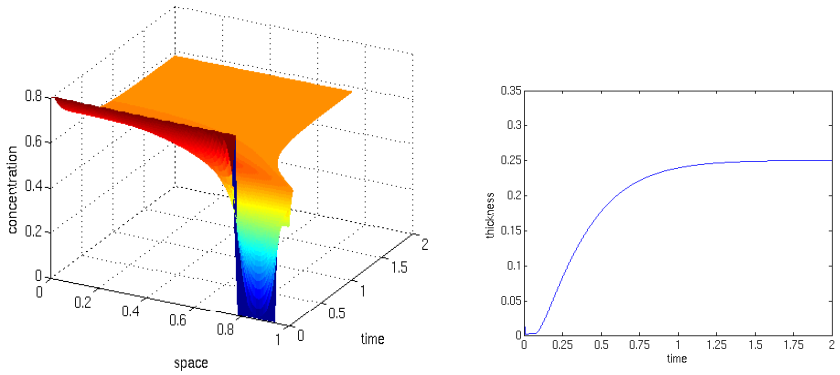


FIG. 5.2. *Results for the second experiment, left plot: the evolution of the concentration $v$ in time displayed in the original coordinates; right plot: the thickness of the crystal layer $h(t)$ versus time.*

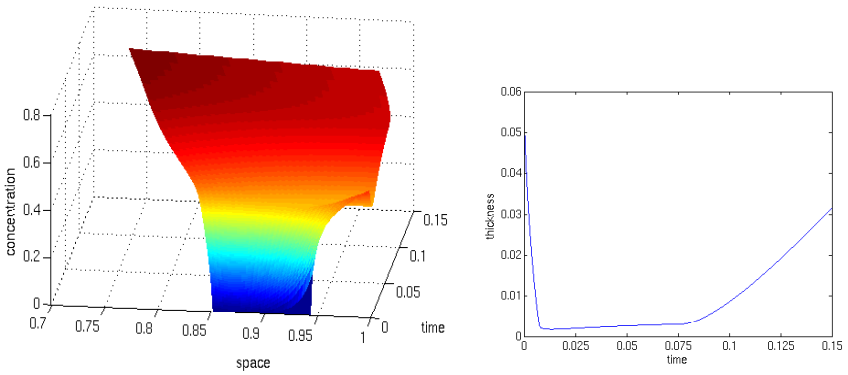


FIG. 5.3. *Results for second experiment, left plot: zoomed in concentration $v$ versus time and space in the original coordinates; right plot: the thickness of the crystal layer $h(t)$ versus time.*

because initially the ion concentration near the crystal layer is small the layer dissolves in a small fraction of one time unit. By diffusion the ion concentration near the boundary increases, and when the ion concentration at the interface exceeds $u^* \approx 0.577$, the crystal layer starts to grow again, until a steady state is reached. At the steady state the ion concentration equals uniformly $u^* \approx 0.577$.

In Figure 5.3, we zoom in near the interface and show also only the initial evolution of the solution. Here we clearly see that the crystal layer first dissolves before it starts growing again.

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**Appendix A. Initial data and compatibility conditions for the regularized problem.** In Section 3.1 we have defined $u_{0,\delta}$ in the following way

$$u_{0,\delta} := \begin{cases} u_0 & \text{if } h_0 < 1 \text{ or } u_0(0) \le v_*, \\ C_\delta u_0 & \text{if } h_0 = 1 \text{ and } v_* < u_0(0) \le v^*, \\ c_\delta u_0 & \text{if } h_0 = 1 \text{ and } u_0(0) > v^*. \end{cases} \tag{A.1}$$

Further $u_{0,\delta}$ should satisfy the compatibility conditions

$$\begin{cases} u_{0,\delta} \in C^2([0,h_1]), \quad \partial_y u_{0,\delta}(h_1) = 0, \\ \partial_y u_{0,\delta}(0) = k\left(r(u_{0,\delta}(0)) - H_\delta\left(1 - \int_0^{h_1} f(u_{0,\delta}(y))dy\right)\right). \end{cases} \tag{A.2}$$

This gives the following equations for $C_\delta$ and $c_\delta$

$$\begin{aligned} 1 - \int_0^{h_1} f(C_\delta u_0)dy &= \delta\, r\big(C_\delta u_0(0)\big), \\ 1 - \int_0^{h_1} f(c_\delta u_0)dy &= \delta\, r\big(c_\delta u_0(0)\big) - \delta\, c_\delta\big(r\big(u_0(0)\big) - 1\big). \end{aligned}$$

The existence of solutions to these equations is the subject of the following two lemmas.

LEMMA A.1. *Let $u_0(0) > v_*$. For all $\delta > 0$, there exists a $C_\delta \in (0,1]$ such that*

$$1 - \int_0^{h_1} f(C_\delta u_0)dy = \delta\, r\big(C_\delta u_0(0)\big).$$

*Moreover $C_\delta \nearrow 1$ for $\delta \searrow 0$.*

*Proof.* Define the function

$$g(C,\delta) := 1 - \int_0^{h_1} f(Cu_0)dy - \delta\, r\big(Cu_0(0)\big). \tag{A.3}$$

For $0 \le C \le 1$ and $\delta \ge 0$, the function $g$ is continuous in both arguments. In addition it follows from the definition of $f$ that there is a $m > 0$ with $\partial_C g \le -m < 0$. Since $h_0 = \int_0^{h_1} f(u_0)dy = 1$, it holds that $g(1,\delta) = 1 - \int_0^{h_1} f(u_0)dy - \delta\, r(u_0(0)) = -\delta\, r(u_0(0))$. Because $u_0(0) > v_*$, it follows that $g(1,\delta) < 0$ for $\delta > 0$. We also have $g(0,\delta) = 1 - \frac{h_1}{\rho} \ge 0$. By the intermediate value theorem and the strict monotonicity of $g$, there exists for all $\delta > 0$ a unique $C_\delta \in (0,1)$ with $g(C_\delta,\delta) = 0$. Furthermore we have that $g(1,\delta) \nearrow 0$ for $\delta \searrow 0$. From the bound on $\partial_C g$ it follows that $C_\delta \nearrow 1$. □

Using similar arguments, we can prove the following lemma.

LEMMA A.2. *Let $u_0(0) > v^*$. For all $\delta > 0$, there exists a $c_\delta \in (0,1]$ such that*

$$1 - \int_0^{h_1} f(c_\delta u_0) dy = \delta\, r\big(c_\delta u_0(0)\big) - \delta\, c_\delta \big(r\big(u_0(0)\big) - 1\big).$$

*Moreover $c_\delta \nearrow 1$ for $\delta \searrow 0$.*

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