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ON AN INTERFACE PROBLEM WITH A NONLINEAR JUMP CONDITION, NUMERICAL APPROXIMATION OF SOLUTIONS

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This paper is dedicated to Max Gunzburger, a teacher and a friend, on the occasion of his 60th birthday.

Abstract. In this paper we describe a one-dimensional interface problem for the heat equation, with a nonlinear (quadratic) jump condition at the interface. We derive a numerical method for approximating solutions of this nonlinear problem and provide some results from numerical experiments. The novelty of this problem is precisely this nonlinear (quadratic) jump condition, and it arises in the study of polymeric ion-selective electrodes and ion sensors.

Key Words. Interface problem, jump condition, ion-selective electrodes.

1. Introduction

In this note we describe a one-dimensional interface problem with a nonlinear jump condition and derive a numerical method for approximating its solutions. This problem arises in the study of polymeric membrane, ion-selective electrodes and ion sensors. The novelty of this problem is precisely this nonlinear (quadratic) jump condition, to our knowledge such problems have not been previously studied.

1.1. The problem. The problem under consideration is a simple, one-dimensional, transmission problem for the heat equation with a nonlinear (quadratic) jump condition at the interface.

Define $\Omega^- = (-1, 0)$, $\Omega^+ = (0, 1)$, and set $\Omega = \Omega^- \cup \Omega^+$. The interface separating the two sub-domains is $\Gamma = \{0\}$. Given a function $u : \Omega \mapsto \mathbb{R}$, we denote its restriction to each of the two sub-domains by $u^\kappa = u|_{\Omega^\kappa}$ for $\kappa = -$, or $\kappa = +$, and by $u(0^\kappa)$ the trace $u^\kappa(0) = u^\kappa|_\Gamma$ of u^κ on Γ.

The model problem we consider is the following transmission problem

$$\frac{1}{\delta} u_t - (k u_x)_x = f \qquad \text{in } \Omega \times (0, T) \tag{1}$$

subject to the boundary conditions

$$u(-1, t) = u_{b^-}(t) \quad \text{and} \quad u(1, t) = u_{b^+}(t) \qquad \text{in } (0, T)\,, \tag{2}$$

initial condition

$$u(x, 0) = u_0(x) \qquad \text{in } \Omega\,, \tag{3}$$

along with the jump conditions (interface conditions, at the interface $x = 0$); a continuity of flux condition

$$k(0^-) u_x(0^-, t) - k(0^+) u_x(0^+, t) = 0 \qquad \text{in } (0, T)\,, \tag{4}$$

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and a nonlinear jump condition

$$\sigma^- u(0^-,t) - \sigma^+ u(0^+,t) = \sigma u(0^-,t)u(0^+,t) \qquad \text{in } (0,T)\,. \tag{5}$$

Here σ^-, σ^+, and σ are positive constants (obviously in the case that σ and/or one of the σ^κ is zero the jump condition becomes linear and the problem greatly simplified, this is also the case if $\sigma^- = \sigma^+ = 0$). While in general k and f may be some given functions, in the case of interest k is a given piecewise constant function

$$k(x) = \begin{cases} k^- & \text{for } x \in \Omega^- \\ k^+ & \text{for } x \in \Omega^+ \end{cases},$$

for some positive constants k^- and k^+, δ is a given piecewise constant

$$\delta(x) = \begin{cases} \delta^- & \text{for } x \in \Omega^- \\ \delta^+ & \text{for } x \in \Omega^+ \end{cases},$$

for some positive constants δ^- and δ^+, and $f = 0$.

1.2. Motivation. The motivation for studying this problem comes from the modeling of chemical sensors which are comprised, in part, of a polymeric membrane, ion-selective, electrode. The model describes the concentration u of an ion I in an aqueous solution (sample) and in an adjoining polymeric membrane, the interface being the point at which the membrane contacts the solution, see [5] and [4] for details. A general description of the operating principle, as well as a simpler model, of such ion sensors may be found in [1].

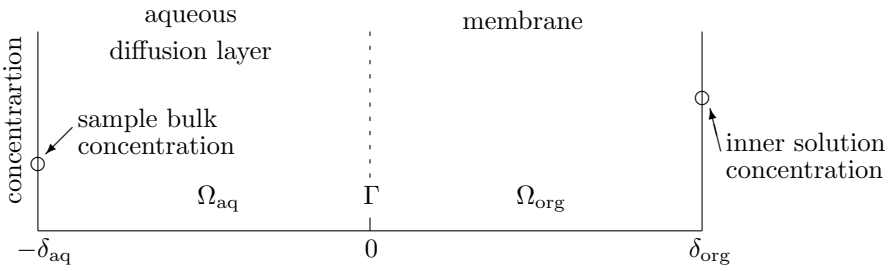

FIGURE 1. The domain, subdomains $\Omega_{\rm aq}$ and $\Omega_{\rm org}$, and interface Γ.

Figure 1 shows the diffusion layer in the aqueous solution $\Omega_{\rm aq} = (-\delta_{\rm aq}, 0)$ which has a width $\delta_{\rm aq}$, and the (organic) membrane $\Omega_{\rm org} = (0, \delta_{\rm org})$ of thickness $\delta_{\rm org}$.

In the absence of sources or sinks the diffusion of ions in the aqueous solution and membrane is governed by

$$u_t - (ku_x)_x = 0 \qquad \text{in } \Omega \times (0,T) \tag{6}$$

where now $\Omega = \Omega_{\rm aq} \cup \Omega_{\rm org}$ (using notation similar to that introduced in the previous section). The ion concentration satisfies the boundary conditions

$$u(-\delta_{\rm aq}, t) = u_{b\ {\rm aq}}(t) \quad \text{and} \quad u(\delta_{\rm org}, t) = u_{b\ {\rm org}}(t) \qquad \text{in } (0,T) \tag{7}$$

where the first condition is given by the sample bulk concentration, and the second is given by the ion concentration in the, so-called, inner solution (a reference solution on the other side of the membrane, see [1]), and the initial condition

$$u(x,0) = u_0(x) \qquad \text{in } \Omega\,. \tag{8}$$

Ion flux continuity across the interface (at $x = 0$) gives rise to the first interface condition

$$k_{\rm aq} u_x(0^-, t) - k_{\rm org} u_x(0^+, t) = 0 \qquad \text{in } (0, T) \tag{9}$$

here

$$k(x) = \begin{cases} k_{\rm aq} & \text{for } x \in \Omega_{\rm aq} \\ k_{\rm org} & \text{for } x \in \Omega_{\rm org} \end{cases}$$

where $k_{\rm aq}$ and $k_{\rm org}$ are the diffusion coefficients in the aqueous solution (the diffusion layer in the sample) and in the membrane respectively.

The concentration relationship at the sample-membrane interface is derived from ion-exchange equilibrium (for such membranes). For analyte ions I that partially exchange at the interface with interfering ions J of the same valency, we have

$$K_{\rm I,J}^{\rm pot} = \frac{u_{\rm aq}(0,t)[u_{\rm R\ org} - u_{\rm org}(0,t)]}{u_{\rm org}(0,t) u_{\rm J\ aq}}$$

where $K_{\rm I,J}^{\rm pot}$ is an experimentally accessible selectivity coefficient (which is here equal to an ion-exchange constant) and $u_{\rm J\ aq}$, $u_{\rm R\ org}$ are the concentrations of interfering ion J in the aqueous phase and in the ion-exchanger in the organic phase, respectively. These concentrations are high and therefore considered constant. This condition may be rewritten as

$$u_{\rm R\ org} u_{\rm aq}(0,t) - K_{\rm I,J}^{\rm pot} u_{\rm J\ aq} u_{\rm org}(0,t) = u_{\rm aq}(0,t) u_{\rm org}(0,t)$$

which can be written (with the obvious substitutions) as

$$\sigma_{\rm aq} u(0^-, t) - \sigma_{\rm aq} u(0^+, t) = \sigma u(0^-, t) u(0^+, t) \qquad \text{in } (0, T)\,. \tag{10}$$

Obviously (6)–(10) (posed on $(-\delta_{\rm aq}, 0) \cup (0, \delta_{\rm org})$) can be transformed to (1)–(5) (posed on $(-1, 0) \cup (0, 1)$) by scaling each interval, as well as k (and f in case it is not zero) appropriately. We can further scale $u_{\rm aq}$ and u_{b^-} by $\sigma_{\rm aq}$, and $u_{\rm org}$ and u_{b^+} by $\sigma_{\rm org}$, so that in (5) we get $\sigma^- = \sigma^+ = 1$; this requires setting

$$k(x) = \begin{cases} \frac{k_{\rm aq}}{\delta_{\rm aq}\sigma_{\rm aq}} & \text{for } x \in \Omega^- \\ \\ \frac{k_{\rm org}}{\delta_{\rm org}\sigma_{\rm org}} & \text{for } x \in \Omega^+ \end{cases},$$

$$\delta(x) = \begin{cases} \delta_{\rm aq}\sigma_{\rm aq} & \text{for } x \in \Omega^- \\ \delta_{\rm org}\sigma_{\rm org} & \text{for } x \in \Omega^+ \end{cases},$$

in (1) and in (4), and replacing σ by $\frac{\sigma}{\sigma_{\rm aq}\sigma_{\rm org}}$ in (5).

2. Theoretical considerations

In light of the above (possible scaling) and in order to focus attention on the distinct features of this model we consider the following slightly simplified problem

$$u_t - (k u_x)_x = f \qquad \text{in } \Omega \times (0, T) \tag{11}$$

subject to the boundary conditions

$$u(-1, t) = u_{b^-}(t) \quad \text{and} \quad u(1, t) = u_{b^+}(t) \qquad \text{in } (0, T)\,, \tag{12}$$

initial condition

$$u(x, 0) = u_0(x) \qquad \text{in } \Omega\,, \tag{13}$$

along with the interface conditions

$$k(0^-)u_x(0^-,t) - k(0^+)u_x(0^+,t) = 0 \qquad \text{in } (0,T)\,, \tag{14}$$

and

$$u(0^-,t) - u(0^+,t) = \sigma u(0^-,t)u(0^+,t) \qquad \text{in } (0,T)\,. \tag{15}$$

Here u_{b^-}, u_{b^+}, and u_0 are piecewise smooth functions, σ is a positive constant, k is a sufficiently regular, positive function (bounded away from zero) or is a given piecewise constant

$$k(x) = \begin{cases} k^- & \text{for } x \in \Omega^- \\ k^+ & \text{for } x \in \Omega^+ \end{cases}$$

for some positive constants k^- and k^+.

We comment that existence and uniqueness of solutions to (11)–(15) are open questions, the difficulty, obviously stemming from the nonlinear jump condition (15). In the sequel we will assume that (11)–(15) has a solution in $C(0,T;H(\Omega))$, where

$$H(\Omega) = \{v \in L^2(\Omega) : v^- \in H^1(\Omega^-) \text{ and } v^+ \in H^1(\Omega^+)\}\,.$$

As usual L^2 is the space of square integrable functions and H^1 is the Sobolev space of square integrable functions whose first distributional derivative is square integrable. We will also make use of the spaces

$$H_0(\Omega) = \{v \in H(\Omega) : v^-(-1) = 0 \text{ and } v^+(1) = 0\}\,,$$
$$H_c(\Omega) = \{v \in H(\Omega) : v^-(0) = v^+(0)\}\,,$$

and

$$H_{0\,c} = H_0(\Omega) \cap H_c(\Omega)\,.$$

That is, $H_0(\Omega)$ is the subspace of $H(\Omega)$-functions with homogeneous boundary conditions and $H_c(\Omega)$ is the subspace of $H(\Omega)$-functions which are continuous at the interface (note that in fact $H_c(\Omega) = H^1(\Omega)$ and $H_{0\,c} = H_0^1(\Omega)$).

2.1. The steady problem. We briefly look at the corresponding steady state problem, this may provide some additional insight and motivation for the numerical algorithm we derive. Consider

$$-(ku_x)_x = f \qquad \text{in } \Omega \tag{16}$$

subject to the boundary conditions

$$u(-1) = u_{b^-} \quad \text{and} \quad u(1) = u_{b^+}\,, \tag{17}$$

along with the interface conditions

$$k(0^-)u_x(0^-) - k(0^+)u_x(0^+) = 0\,, \tag{18}$$

and

$$u(0^-) - u(0^+) = \sigma u(0^-)u(0^+)\,, \tag{19}$$

with k as before.

It is a fairly simple exercise to show that (16)–(19) has two solutions in $H(\Omega)$ provided that $\sigma \neq 0$.

2.2. Auxiliary problem. Also consider the auxiliary problem

$$-(kw_x)_x = 0 \qquad \text{in } \Omega \tag{20}$$

subject to the boundary conditions

$$w(-1) = 0 \quad \text{and} \quad w(1) = 0\,, \tag{21}$$

along with the interface conditions

$$k(0^-)w_x(0^-) - k(0^+)w_x(0^+) = 0\,, \tag{22}$$

and

$$w(0^-) - w(0^+) = \sigma\,, \tag{23}$$

with k as before.

With $\sigma = 0$ in (19) problem (16)–(19) becomes a standard linear transmission problem (with zero jump), hence it is easy to show that it has a unique solution $v \in H_c(\Omega)$. Furthermore (20)–(23) is also a linear transmission problem (with a nonzero jump condition), hence it too has a unique solution $w \in H_0(\Omega)$.

Now consider $u = v + \beta w$. If β is a root of

$$\begin{aligned} 0 &= (\beta w(0^-) + v(0))(\beta w(0^+) + v(0)) - \beta \\ &= w(0^-)w(0^+)\beta^2 + [(w(0^-) + w(0^+))v(0) - 1]\beta + v^2(0) \end{aligned} \tag{24}$$

(recall v is continuous at $x = 0$) then $u = v + \beta w$ is in $H(\Omega)$ and is a solution of (16)–(19). It is easily seen that the quadratic (24) always has two real solutions (since $w(0^-)w(0^+) < 0$, see below; furthermore one root is negative and the other nonnegative). The above construction does not require that $f \neq 0$ or that k be piecewise constant. Hence (16)–(19) has two solutions.

We further observe that w can be written as

$$w(x) = \sigma \left\| \frac{1}{k} \right\|_{L^1}^{-1} \begin{cases} \int_{-1}^{x} \frac{d\xi}{k(\xi)} & \text{for } x \in \Omega^- \\ \\ -\int_{x}^{1} \frac{d\xi}{k(\xi)} & \text{for } x \in \Omega^+ \end{cases}.$$

In the physical case, that is when $f = 0$ and k is a piecewise constant, we have the explicit expressions

$$v(x) = \begin{cases} u_{b^-} + \frac{k^+}{(k^- + k^+)}(u_{b^+} - u_{b^-})(x+1) & \text{for } x \in \Omega^- \\ \\ u_{b^+} + \frac{k^-}{(k^- + k^+)}(u_{b^+} - u_{b^-})(x-1) & \text{for } x \in \Omega^+ \end{cases}$$

and

$$w(x) = \begin{cases} \frac{\sigma k^+}{(k^- + k^+)}(x+1) & \text{for } x \in \Omega^- \\ \\ \frac{\sigma k^-}{(k^- + k^+)}(x-1) & \text{for } x \in \Omega^+ \end{cases}.$$

In this physical case it can be shown that one solution is nonnegative on Ω, we call it the physical solution, whereas the second solution is negative somewhere in Ω, we call it the non-physical solution (in the applications we have in mind, u is a concentration, hence must be nonnegative).

3. Numerical approximation of solutions

We now describe the numerical method (finite element in space, finite difference in time, see, e.g., [2] or [3] for an introduction to these methods) that we use to approximate solutions of (11)–(15), the one-dimensional transmission problem with a nonlinear jump condition.

We start by writing a weak form for the differential equation which is obtained as usual, multiplying (11) by a test function $v \in H_{0\,c}(\Omega)$ and integrating by parts. The weak formulation is, find $u \in H(\Omega)$ which satisfies the boundary conditions (12), the initial condition (13), the jump condition (15), and such that

$$\int_{-1}^{1} [u_t v + k u_x v_x]\, dx = \int_{-1}^{1} f v\, dx \qquad \text{for all } v \in H_{0\,c}(\Omega) \text{ and a.e. } t \in (0,T)\,. \tag{25}$$

Note the interface condition (14) is incorporated into the weak form (is a natural condition and does not have to be explicitly enforced).

To perform the actual numerical simulation we discretize the weak form (25), to that end we generate a mesh in the interval $[-1,1]$, that is, subdivide the interval into $l+r$ sub-intervals (elements) with (end points)

$$-1 = x_{-l} < x_{-l+1} < \ldots < x_0 = 0 < x_1 < \ldots < x_{r-1} < x_r = 1\,.$$

On this grid we construct some finite element spaces. Here we used piecewise linear basis functions, see Figure 2.

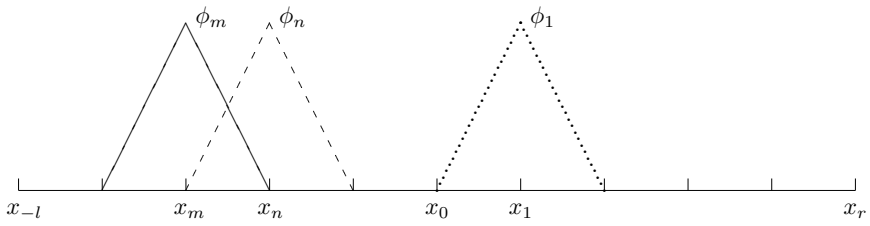

FIGURE 2. The grid and basis functions.

We denote by ϕ_m, $-l \le m \le r$, the piecewise linear functions given by

$$\phi_m(x_n) = \begin{cases} 1 & \text{for } m = n \\ \\ 0 & \text{for } m \neq n \end{cases} \qquad -l \le m, n \le r\,.$$

We in fact construct three finite element spaces, the (trial) space $V^h \subset H(\Omega)$, the (continuous) space $V_c^h \subset H_c(\Omega)$, and the (test) space $V_{0\,c}^h = V_c^h \cap H_0(\Omega) \subset H_{0\,c}(\Omega)$. The bases for these three spaces are given by $\{\phi_m : -l \le m \le r, m \neq 0\} \cup \{\phi_0^-, \phi_0^+\}$, $\{\phi_m : -l \le m \le r\}$, and $\{\phi_m : -l+1 \le m \le r-1\}$, respectively.

The semi-discrete (piecewise linear in space continuous in time) approximation $u^h \in C(0,T;V^h)$ of a function $u \in C(0,T;H(\Omega))$ may be written as

$$u^h(x,t) = \sum_{\substack{m=-l \\ m\neq 0}}^{r} u_m^h(t)\phi_m(x) + u_0^{h\,-}(t)\phi_0^-(x) + u_0^{h\,+}\phi_0^+(x) \tag{26}$$

where u_m^h are some continuous functions, and a function $v^h \in V_{0c}^h$ may be written as

$$v^h(x) = \sum_{m=-l+1}^{r-1} v_m^h \phi_m(x) \tag{27}$$

for some coefficients v_m^h. We note that the function v^h is continuous across the interface, whereas u^h may have a jump discontinuity there due to the two (possibly) different functions $u_0^{h\,-}$ and $u_0^{h\,+}$ multiplying ϕ_0^- and ϕ_0^+, the restrictions of ϕ_0 to Ω^- and Ω^+ respectively. We also point out that the coefficients v_m^h and (functions of time) u_m^h are the nodal values (values at the grid points) of v^h and u^h respectively.

We now also introduce time nodes; set $\Delta t = \frac{T}{s}$, for some integer s, and let $t_j = j\Delta t$, for $0 \le j \le s$.

We discretize the weak form of the p.d.e. (25) using these piecewise linear finite elements in space and finite differences in time to obtain the discrete equation for the approximate solution

$$\begin{aligned} \int_{-1}^{1} \Bigg\{ & \frac{u^h(x,t_{j+1}) - u^h(x,t_j)}{\Delta t} v^h(x) \\ & + k(x) \left[\omega u_x^h(x,t_{j+1}) + (1-\omega) u_x^h(x,t_j) \right] v_x^h(x) \Bigg\} dx \\ = & \int_{-1}^{1} [\omega f(x,t_{j+1}) + (1-\omega) f(x,t_j)] v^h(x)\, dx \\ & \qquad \text{for all } v^h \in V_{0c}^h \text{ and } 0 \le j \le s-1 \end{aligned} \tag{28}$$

subject to the boundary conditions

$$u^h(-1,t_{j+1}) = u_{b^-}(t_{j+1}) \quad \text{and} \quad u^h(1,t_{j+1}) = u_{b^+}(t_{j+1}) \qquad \text{for } 0 \le j \le s-1\,,$$

the initial condition

$$u^h(x,t_0) = w_0^h(x) \qquad \text{in } \Omega\,,$$

where w_0^h is some V^h approximate of u_0, and the interface condition

$$u^h(0^-,t_{j+1}) - u^h(0^+,t_{j+1}) = \sigma u^h(0^-,t_{j+1}) u^h(0^+,t_{j+1}) \qquad \text{for } 0 \le j \le s-1\,.$$

In equation (28) setting $\omega = 0$, $1/2$, and 1 yields the Euler, Crank-Nicolson, and backward Euler methods, respectively (see, for example, [2] or [3]).

Using (26), (27) and (28) we get, for each $0 \le j \le s-1$ an equivalent system of linear algebraic equations

$$
\begin{aligned}
&\int_{-1}^{1} \Bigg\{ \Bigg(\sum_{\substack{m=-l \\ m\neq 0}}^{r} \frac{u_m^h(t_{j+1}) - u_m^h(t_j)}{\Delta t}\phi_m(x) + \frac{u_0^{h\,-}(t_{j+1}) - u_0^{h\,-}(t_j)}{\Delta t}\phi_0^-(x) \\
&\qquad + \frac{u_0^{h\,+}(t_{j+1}) - u_0^{h\,+}(t_j)}{\Delta t}\phi_0^+(x) \Bigg)\phi_n(x) \\
&\qquad + \Bigg[\omega k(x) \Bigg(\sum_{\substack{m=-l \\ m\neq 0}}^{r} u_m^h(t_{j+1})\phi_{m\,x}(x) + u_0^{h\,-}(t_{j+1})\phi_{0\;x}^-(x) + u_0^{h\,+}(t_{j+1})\phi_{0\;x}^+(x) \Bigg) \\
&\qquad + (1-\omega)k(x) \Bigg(\sum_{\substack{m=-l \\ m\neq 0}}^{r} u_m^h(t_j)\phi_{m\,x}(x) + u_0^{h\,-}(t_j)\phi_{0\;x}^-(x) + u_0^{h\,+}(t_j)\phi_{0\;x}^+(x) \Bigg) \Bigg] \\
&\qquad \times \phi_{n\,x}(x) \Bigg\}\, dx = \int_{-1}^{1} [\omega f(x,t_{j+1}) + (1-\omega) f(x,t_j)]\phi_n(x)\, dx \\
&\qquad\qquad \text{for } -l+1 \le n \le r-1 \text{ and } 0 \le j \le s-1\,.
\end{aligned} \tag{29}
$$

Note, after using the initial condition

$$u_m^h(t_0) = w_0^h(x_m) \qquad \text{for } -l \le m \le r\,,$$

at each time step (for each $0 \le j \le s-1$) (29) is a system of $r+l-1$ equations in $r+l+2$ unknowns, moreover, the boundary conditions

$$u_{-l}^h(t_{j+1}) = u_{b^-}(t_{j+1}) \quad \text{and} \quad u_r^h(t_{j+1}) = u_{b^+}(t_{j+1}) \qquad \text{for } 0 \le j \le s-1 \tag{30}$$

add two additional linear equations, and the jump condition

$$u_0^{h\,-}(t_{j+1}) - u_0^{h\,+}(t_{j+1}) = \sigma u_0^{h\,-}(t_{j+1}) u_0^{h\,+}(t_{j+1}) \qquad \text{for } 0 \le j \le s-1 \tag{31}$$

adds an additional nonlinear (algebraic equation) constraint. These can be written as

$$
\begin{aligned}
M\mathbf{u}^h(t_{j+1}) + \omega\Delta t S\mathbf{u}^h(t_{j+1}) &= M\mathbf{u}^h(t_j) - (1-\omega)\Delta t S\mathbf{u}^h(t_j) \\
&\quad + \Delta t[\omega\mathbf{f}(t_{j+1}) + (1-\omega)\mathbf{f}(t_j)] \qquad \text{for } 0 \le j \le s-1\,,
\end{aligned} \tag{32}
$$

with boundary conditions

$$u_{-l}^h(t_{j+1}) = u_{b^-}(t_{j+1}) \quad \text{and} \quad u_r^h(t_{j+1}) = u_{b^+}(t_{j+1}) \qquad \text{for } 0 \le j \le s-1\,, \tag{33}$$

jump condition

$$u_0^{h\,-}(t_{j+1}) - u_0^{h\,+}(t_{j+1}) = \sigma u_0^{h\,-}(t_{j+1}) u_0^{h\,+}(t_{j+1}) \qquad \text{for } 0 \le j \le s-1\,, \tag{34}$$

and initial condition

$$\mathbf{u}^h(t_0) = \mathbf{w}_0^h\,.$$

Here M is the mass matrix, S the stiffness matrix, $\mathbf{u}^h$ the vector of nodal values, $\mathbf{f}$ the load vector, and $\mathbf{w}_0^h$ the vector of initial values at the nodes .

Since the above discretization yields a system of algebraic equations coupled to a nonlinear equation (constraint) we developed an efficient analytic and numerical procedure for solving such a problem. The method for solving the problem involves a *splitting*, that is constructing the solution by superposing a solution of the nonhomogeneous equation with a zero jump and a solution that satisfies the corresponding homogeneous equation with a prescribed jump. The approach is similar in spirit to that described in section 2 (in the p.d.e. context, and for a quadratic jump does not require iteration).

Consider solving the linear algebraic system

$$A\mathbf{u} = \mathbf{b}$$

where A is the matrix corresponding to the system of linear algebraic equations (32) and the two linear equations (33) representing the boundary conditions. The vector $\mathbf{u}$ is the vector of nodal (unknown) values of u^h, that is a vector whose components are u^h_m (at some time t_j), and the vector $\mathbf{b}$ is the right hand side of this linear system. We must solve this linear system along with the (possibly nonlinear) constraint which corresponds here to the jump condition (34) (represented abstractly as)

$$B(\mathbf{u}) = h\,.$$

We solve this problem in three steps as follows:
i. Solve the linear system with homogeneous constraint

$$A\bar{\mathbf{u}} = \mathbf{b}$$

$$B(\bar{\mathbf{u}}) = 0\,.$$

ii. Solve a homogeneous linear system with constraint 1

$$A\hat{\mathbf{u}} = 0$$

$$B(\hat{\mathbf{u}}) = 1\,.$$

iii. Finally find β such that

$$B(\bar{\mathbf{u}} + \beta\hat{\mathbf{u}}) = h\,.$$

If these three systems of equations can be solved then, it is easy to see that $\mathbf{u} = \bar{\mathbf{u}} + \beta\hat{\mathbf{u}}$ is a solution to our problem, this is represented schematically (for the case of piecewise constant k and $f = 0$) in Figure 3.

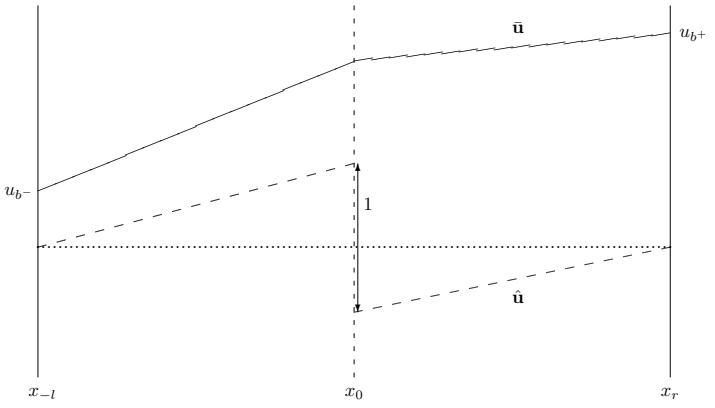

FIGURE 3. The solutions $\bar{\mathbf{u}}$ and $\hat{\mathbf{u}}$; building blocks for obtaining the solution $\mathbf{u}$.

To obtain an approximate solution of the interface problem we solve such a system at each time step. In this case finding β amounts to computing the roots of a quadratic polynomial (24) and choosing the appropriate root (which yields the physical solution).

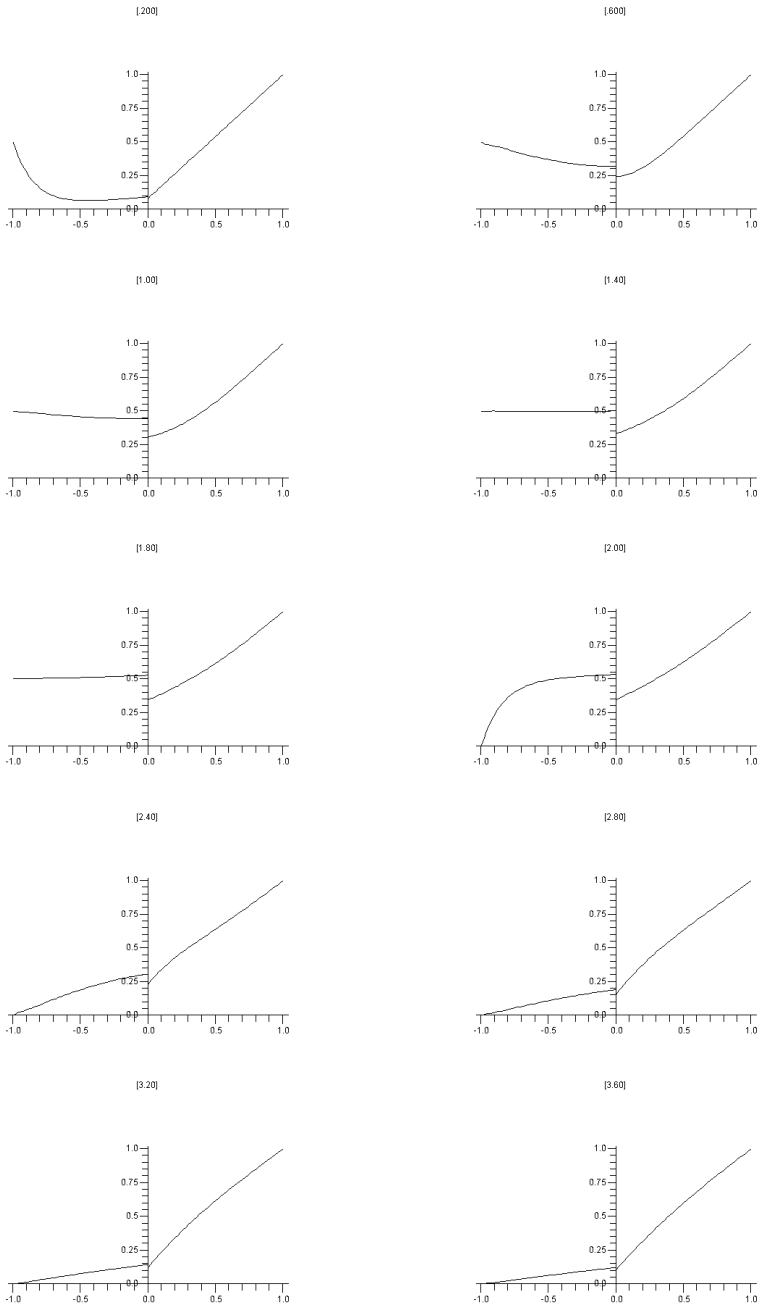

FIGURE 4. Example 1, concentration snapshots for $t = 0.2$, 0.6, 1.0, 1.4, 1.8, 2, 2.4, 2.8, 3.2, and 3.6.

4. Numerical experiments

We now describe computational results from two computer experiments. These results provide additional insight into the behavior of solutions of the model problem (11)–(15).

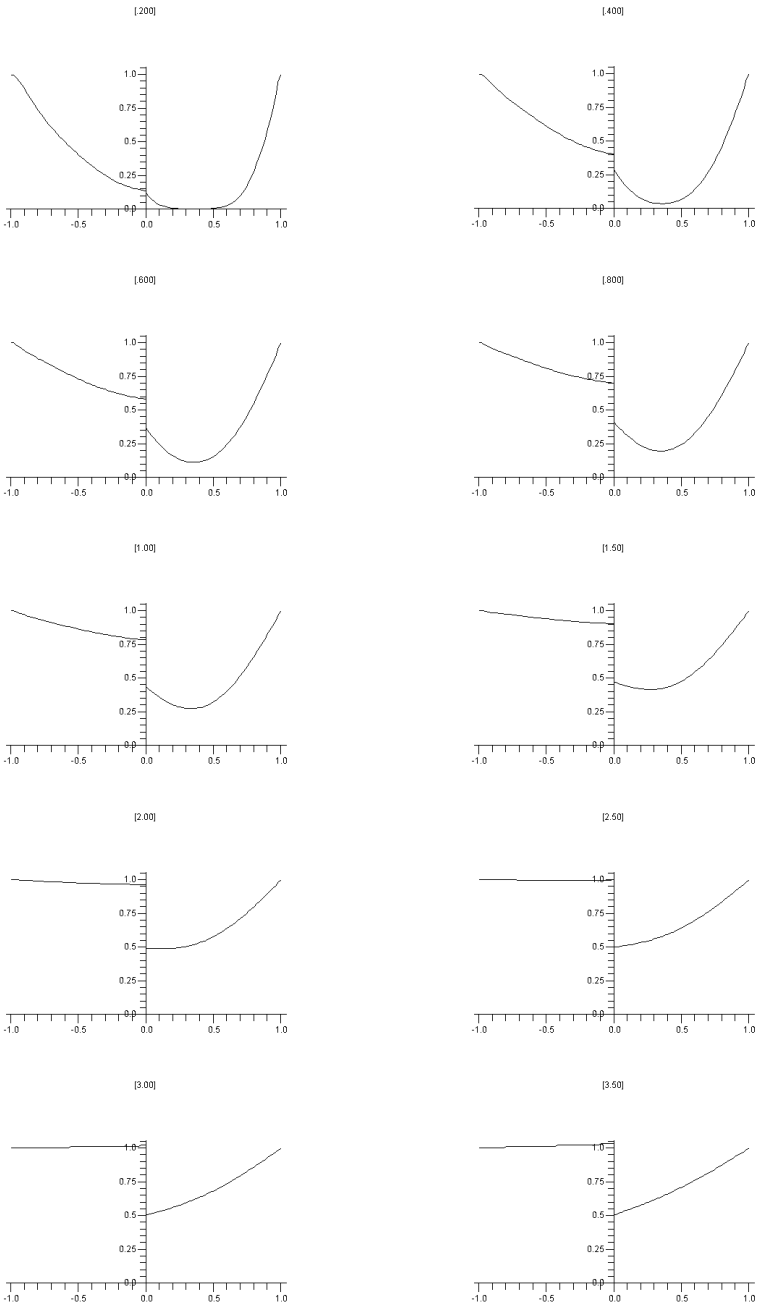

FIGURE 5. Example 2, concentration snapshots for $t = 0.2$, 0.4, 0.6, 0.8, 1, 1.5, 2, 2.5, 3, and 3.5.

In these examples we used the Crank-Nicolson method (that is $\omega = 1/2$ in (28)). For both examples we chose $k^- = 1$, $k^+ = 0.1$, and $\sigma = 1$. The first example resembles chemistry experiments (see [5] and [4]). The initial condition is the

steady state for $u_{b^-} = 0$ and $u_{b^+} = 1$, that is

$$u(x,0) = \begin{cases} \frac{-5+\sqrt{35}}{10}(x+1) & \text{for } x \in \Omega^- \\ \\ 1-(5-\sqrt{35})(x-1) & \text{for } x \in \Omega^+ \end{cases} .$$

At time $t = 0.2$ the concentration in the sample is increased, to 0.5 and at time $t = 2$ the concentration in the sample is decreased back to zero, that is

$$u_{b^-}(t) = \begin{cases} 0 & \text{for } 0 < t < 0.2 \\ 0.5 & \text{for } 0.2 < t < 2 \\ 0 & \text{for } 2 < t \end{cases} \quad \text{and} \quad u_{b^+}(t) = 1 \,.$$

Snapshots of the solution u^h (the concentration) at various times are shown in Figure 4.

In Figure 5 we show snapshots of the solution u^h at various times for a more academic example. Here we chose a zero initial condition, that is

$$u(x,0) = 0 \qquad \text{for } x \in \Omega$$

and at time zero both the sample concentration and inner solution concentration are raised to 1, that is

$$u_{b^-}(t) = 1 \quad \text{and} \quad u_{b^+}(t) = 1 \qquad \text{in } (0,T) \,.$$

While here we only considered *academic* numerical experiments, there is good agreement between results of numerical simulation and laboratory experiments. Such comparisons may be found in [5] and [4].

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