

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

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

subject to the boundary conditions

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

initial condition

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

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

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

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and a nonlinear jump condition

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

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].

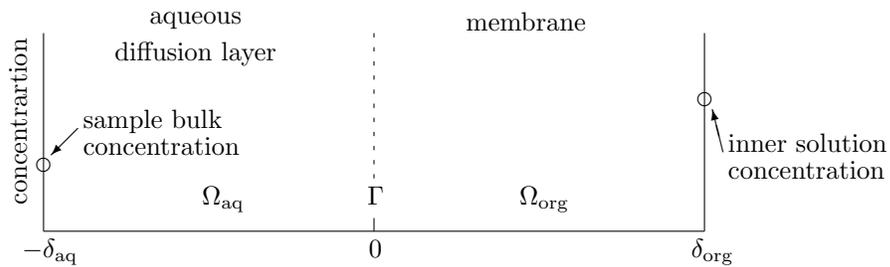


FIGURE 1. The domain, subdomains Ω_{aq} and Ω_{org} , and interface Γ .

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

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

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

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

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

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

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