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The reaction–diffusion problem with dynamical boundary condition

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ABSTRACT

The aim of this paper is to prove the existence and uniqueness of classical solutions to a coupled system of three parabolic and one ordinary differential equations, with the latter determined on the boundary. This system describes the receptor–toxin–antibody interaction problem taking into account diffusion of reacting species.

1. Introduction

In the theory of differential equations, coupled systems of parabolic and ordinary differential equations are usually considered in the same domain (see [1–3], and references therein). The process of the bulk diffusion and heterogeneous chemical reactions can be modeled by a coupled system of parabolic and ordinary differential equations, with the latter considered on the boundary of the domain. Such a coupled system is studied in [4,5], where the existence and uniqueness of classical solutions are established. In [6,7], these problems are considered by numerical methods. Similar models are studied in [8,9]. The unbounded domain case with the plane, spherical, or cylindrical boundary and spherical or cylindrical symmetry, respectively, is considered in [10], where the problem is reduced to a nonlinear Volterra-type integral equation and solved numerically. If the diffusion is possible not only in the domain, but also on some part of its boundary, then we have a system of two coupled parabolic equations, one of which has to be investigated in the domain, while the other one has to be solved on the part of its boundary. Such a coupled system of parabolic equations is investigated in [11], where the existence and uniqueness of classical solutions of the problem are proved. In [12], this problem is solved numerically.

In this paper, we prove the existence and uniqueness theorem of classical solutions to the model proposed and considered numerically in [13] for receptor–toxin–antibody interaction. In this model, a chemical reaction takes place both in the domain and on a part of its boundary. This model is described by a coupled system of three parabolic and one ordinary differential equations.

The paper is organized as follows. In Section 2, we describe the model. In Section 3, we formulate the main results. A priori estimates are given in Section 4. Sections 5 and 6 are devoted to the uniqueness and existence of the classical solution to problem (1)–(4).

2. Formulation of the problem

Suppose that toxin A, antibody B, and toxin–antibody complex C occupy a bounded domain $\Omega \subset \mathbb{R}^n$, $n \geq 3$, with concentrations $a = a(x,t)$, $b = b(x,t)$, and $c = c(x,t)$ of A, B, C, respectively, at point $x \in \Omega$ at time t. Let $S := \partial\Omega \subset C^{1+\alpha}$, $\alpha \in (0,1)$, be a surface of dimension $n-1$, S_2 a closed part of S of the same dimension, and $S_1 = S \setminus S_2$; let $\rho = \rho(x)$

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be the concentration of receptors on the surface S at point $x \in S$, $\rho \in C(S)$, $\rho(x) \geq 0$ for $x \in S$ and $\rho(x) = 0$ for $x \in S_1$, $\theta = \theta(x,t)$ be the fraction of the toxin bound receptors, and $\rho(1-\theta)$ be the concentration of the free receptors of S_2.

According to [13], the reaction–diffusion model for the receptor–toxin–antibody interaction can be described by the following system:

$$\begin{cases} \theta' = \kappa(1-\theta)a - \kappa_1\theta - \kappa_2\theta, & t \in (0,T],\ x \in S_2, \\ \theta|_{t=0} = \theta_0, & x \in S_2, \end{cases} \tag{1}$$

$$\begin{cases} a_t - k_a\Delta a + \kappa_3 ba = \kappa_4 c & \text{in } \Omega \times (0,T), \\ k_a \dfrac{\partial a}{\partial \mathbf{n}} + \kappa\rho(1-\theta)a = \kappa_1\rho\theta & \text{on } S_2 \times (0,T), \\ k_a \dfrac{\partial a}{\partial \mathbf{n}} = 0 & \text{on } S_1 \times (0,T), \\ a|_{t=0} = a_0 & \text{in } \overline{\Omega}, \end{cases} \tag{2}$$

$$\begin{cases} b_t - k_b\Delta b + \kappa_3 ab = \kappa_4 c & \text{in } \Omega \times (0,T), \\ k_b \dfrac{\partial b}{\partial \mathbf{n}} = 0 & \text{on } S \times (0,T), \\ b|_{t=0} = b_0 & \text{in } \overline{\Omega}, \end{cases} \tag{3}$$

$$\begin{cases} c_t - k_c\Delta c + \kappa_4 c = \kappa_3 ab & \text{in } \Omega \times (0,T), \\ k_c \dfrac{\partial c}{\partial \mathbf{n}} = 0, & \text{on } S \times (0,T), \\ c|_{t=0} = c_0 & \text{in } \overline{\Omega}, \end{cases} \tag{4}$$

where:

$\theta' = d\theta/dt$, $a_t = \partial a/\partial t$, $b_t = \partial b/\partial t$, $c_t = \partial c/\partial t$,
Δ is the n-dimensional Laplace operator,
$\partial/\partial\mathbf{n}$ is the outward normal derivative to S,
$a_0 = a_0(x)$, $b_0 = b_0(x)$, and $c_0 = c_0(x)$ are the initial concentrations of A, B, and C, respectively, at point $x \in \overline{\Omega}$,
$\theta_0 = \theta_0(x)$ is the initial value of θ such that $0 \leq \theta_0(x) < 1$ for $x \in S_2$,
k_a, k_b, and k_c are the diffusivities of the toxin, antibody, and toxin–antibody complex,
κ, κ_1 are the forward and reverse constants of the toxin and receptor binding rate,
κ_2 is the toxin internalization rate constant,
κ_3, κ_4 are the forward and reverse constants of the toxin–antibody reaction rate.

All constants $\kappa, \kappa_1, \kappa_2, \kappa_3, \kappa_4$ are assumed to be positive.

3. The main results

Assumption 3.1. S is a surface of class $C^{1+\alpha}$, $\alpha \in (0,1)$.

Assumption 3.2. The functions θ_0, a_0, b_0, c_0, and ρ satisfy the following conditions:

1. the function θ_0 is continuous on S_2, and $0 \leq \theta_0(x) < 1$ for all $x \in \overline{S}_2$,
2. the functions a_0, b_0, and c_0 are continuous and nonnegative in a closed domain $\overline{\Omega}$,
3. $\rho \in C(S)$, $\rho(x) \geq 0$ for all $x \in S$, and $\rho(x) = 0$ for all $x \in S_1$.

Assumption 3.3. The functions a_0, b_0, and c_0 are continuously differentiable on a neighborhood of the surface S.

Definition 3.1. Functions θ, a, b, and c form a classical solution to problem (1)–(4) if $\theta \in C(S_2 \times [0,T])$, $\theta' \in C(S_2 \times (0,T])$, the derivatives $\partial a/\partial\mathbf{n}$, $\partial b/\partial\mathbf{n}$, and $\partial c/\partial\mathbf{n}$ are continuous on $S \times [0,T]$, and $a, b, c \in C^{2,1}(\Omega \times (0,T]) \cap C(\overline{\Omega} \times [0,T])$.

Our main result is the following:

Theorem 3.1. *Let the surface S satisfy Assumption 3.1, and the known functions a_0, b_0, c_0, θ_0, and ρ satisfy Assumptions 3.2 and 3.3. Then problem (1)–(4) has a unique classical solution.*

The proof of this theorem is based on the following four propositions.

Lemma 3.1. *Let function $a = a(x,t)$ be continuous and nonnegative on $S_2 \times [0,T]$, and θ_0 satisfy Assumption 3.2. Let θ be a solution to Cauchy problem (1). Then, for all $x \in S_2$ and $t \in [0,T]$, the following estimates hold:*

$$\theta(x,t) \geq \theta_0(x)e^{-(\kappa_1+\kappa_2)t}e^{-\int_0^t \kappa a(x,s)\,ds} \geq 0,$$

$$\theta(x,t) \leq 1 - (1-\theta_0(x))e^{-\int_0^t \kappa a(x,s)\,ds} < 1.$$