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N.D.Botkin, K.-H.Hoffmann,
A.M.Meirmanov, V.N.Starovoitov

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DIFFUSION PROBLEM WITH BOUNDARY CONDITIONS OF HYSTERESIS TYPE

N.D.BOTKIN, K.-H.HOFFMANN, A.M.MEIRMANOV, V.N.STAROVOITOV

1 Introduction

The problem we consider in this paper appears when developing sensors which serve for detecting of certain proteins in solutions. An important part of such sensors is a wet cell, say a cube, filled with water into which a solution containing the protein to be detected is injected. Special molecules called aptamers are immobilized on the bottom of the wet cell. The aptamers can selectively bind the desired protein from the solution. The change of the surface mass loading can be analyzed using acoustic waves propagating along the aptamer layer. Thus, the concentration of the protein in the solution can be estimated. In this paper, a model that describes the propagation of the protein in the wet cell and its adhering to the aptamer is proposed. It is assumed for simplicity that the propagation of the injected protein in the wet cell is governed by an diffusion equation. A special boundary condition on the bottom provides the monotone grows of the deposited layer with saturation which means the exhaustion of free aptamer molecules.

1.1 The model

Let $\Omega = \{\boldsymbol{x} = (x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_i \in (0,1),\ i = 1,2,3\}$ be the unit open cube in $\mathbb{R}^3$ (the wet cell), $\partial\Omega$ its boundary. Let $\Gamma = \{\boldsymbol{x} \in \mathbb{R}^3 \mid x_3 = 0\}$ be the part of $\partial\Omega$ occupied by aptamers.

Suppose that Ω is filled with a liquid $\mathcal{W}$, and some substance $\mathcal{P}$ is solved there. Let ρ_p and ρ_w be the proper densities of $\mathcal{P}$ and $\mathcal{W}$, respectively. Denote by ϕ the volume concentration and by ρ the mass concentration of the substance $\mathcal{P}$ in Ω. That is, $\rho = \phi\rho_p$. The function ϕ satisfies the equation

$$\frac{\partial \phi}{\partial t} = \operatorname{div} \boldsymbol{j} \qquad \text{in} \quad \Omega, \tag{1.1}$$

where $\boldsymbol{j}$ is the diffusion flux of $\mathcal{P}$ and t is the time variable. Note that the diffusion mass flux is equal to $\rho_p \boldsymbol{j}$. We suppose that

$$\boldsymbol{j} \cdot \boldsymbol{\nu} = 0 \qquad \text{on} \quad \partial\Omega \setminus \Gamma, \tag{1.2}$$

where $\boldsymbol{\nu}$ is the outward normal to $\partial\Omega$. This means that there is no flux of $\mathcal{P}$ through the boundary of Ω except for Γ. The flux of $\mathcal{P}$ can be different from zero due to the aptamers that adhere the substance $\mathcal{P}$ from the solution.

Let us denote by μ the surface mass distribution of $\mathcal{P}$ on Γ. That is μ is the amount of the substance caught by the aptamers per unit area of Γ. Note that its dimension is kg/m^2. We assume the mass conservation of $\mathcal{P}$ so that

$$\frac{\partial \mu}{\partial t} = \rho_p \boldsymbol{j} \cdot \boldsymbol{\nu} \qquad \text{on} \quad \Gamma. \tag{1.3}$$

Let us introduce the surface concentration η of $\mathcal{P}$ on Γ. We denote by Γ_δ the set $\{\boldsymbol{x} \in \mathbb{R}^3 \mid -\delta \le x_3 \le 0,\ (x_1, x_2, 0) \in \Gamma\}$, where δ is a positive number. In fact, the aptamers can be imagine like thin pins which occupy the layer Γ_δ near Γ (see Fig. 1), and the substance $\mathcal{P}$ can diffuse into this layer. We consider a molecule of $\mathcal{P}$ being caught by the aptamers, if it penetrates into this layer. Let us denote by $\bar\phi$ the concentration of molecules of $\mathcal{P}$ caught by the aptamers in Γ_δ. Then

$$\mu = \rho_p \int_{-\delta}^{0} \bar\phi \, dx_3.$$

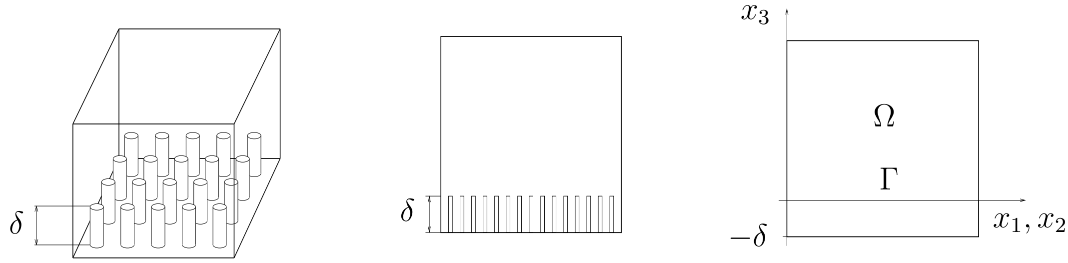


Figure 1: The aptamers layer.

The aptamers can not catch more then a certain amount of molecules of $\mathcal{P}$. After that, the molecules remain in Ω. That is $\bar{\phi}$ can not exceed some positive number $\bar{\phi}_0 \in (0, 1)$. We define the surface concentration η as

$$\eta = \frac{1}{\sigma} \int_{-\delta}^{0} \bar{\phi} \, dx_3,$$

where $\sigma = \bar{\phi}_0 \delta$. Thus, if $\eta = 1$ at some point on Γ, then molecules of $\mathcal{P}$ can not more adhere at this place. If $\eta = 0$ somewhere, then the aptamers are completely free at this place.

It is not difficult to see that the functions η and μ are connected through the relation

$$\mu = \sigma \rho_p \eta,$$

which together with (1.3) gives

$$\sigma \frac{\partial \eta}{\partial t} = \boldsymbol{j} \cdot \boldsymbol{\nu} \qquad \text{on} \quad \Gamma. \tag{1.4}$$

According to the Fick's law,

$$\boldsymbol{j} = -\alpha \nabla \phi, \tag{1.5}$$

where α is a positive constant.In order to complete the statement of the problem, we have to specify a relation between η and ϕ, which will play the role of a constitutive law. Here, we should take into account properties of the aptamer. First of all, if the aptamer catch a molecule, it will be not released. Besides that, there exist two values ϕ_0 and ϕ_1 of the concentration ϕ such that if $\phi \le \phi_0$ near Γ, then the aptamer can not catch molecules of $\mathcal{P}$. On the other hand, if ϕ achieves the value ϕ_1 somewhere, then the aptamer is completely saturated at this place and can not catch molecules any more so that they remain in Ω. We assume that $0 \le \phi_0 < \phi_1$. These properties of the aptamers can be modeled as follows.

Let $H_0(\phi_0, \phi_1, \cdot) : \mathbb{R} \to [0, 1]$ be a Lipschitz continuous non-decreasing function such that $H_0(\phi_0, \phi_1, s) = 0$ if $s \le \phi_0$ and $H_0(\phi_0, \phi_1, s) = 1$ if $s \ge \phi_1$. We introduce an operator $\mathcal{A}_0(\phi_0, \phi_1, \cdot) : L^\infty(0, T) \to L^\infty(0, T)$ such that

$$\mathcal{A}_0(\phi_0, \phi_1, \varphi)(t) = \operatorname*{ess\,sup}_{0 \le \tau \le t} H_0\big(\phi_0, \phi_1, \varphi(\tau)\big)$$

for almost all $t \in [0, T]$ and for all $\varphi \in L^\infty(0, T)$. This is a hysteresis operator, which acts as it is shown schematically in Fig. 2. We postulate the following constitutive law

$$\eta(\boldsymbol{x}, t) = \mathcal{A}_0\big(\phi_0, \phi_1, \phi(\boldsymbol{x}, \cdot)\big)(t) \qquad \text{for} \quad x \in \Gamma, \; t \in [0, T]. \tag{1.6}$$

Equations (1.1), (1.2), (1.4), (1.5), (1.6) form a closed model which can be used for the description of the deposition of a protein in the presence of the corresponding aptamer that adheres and

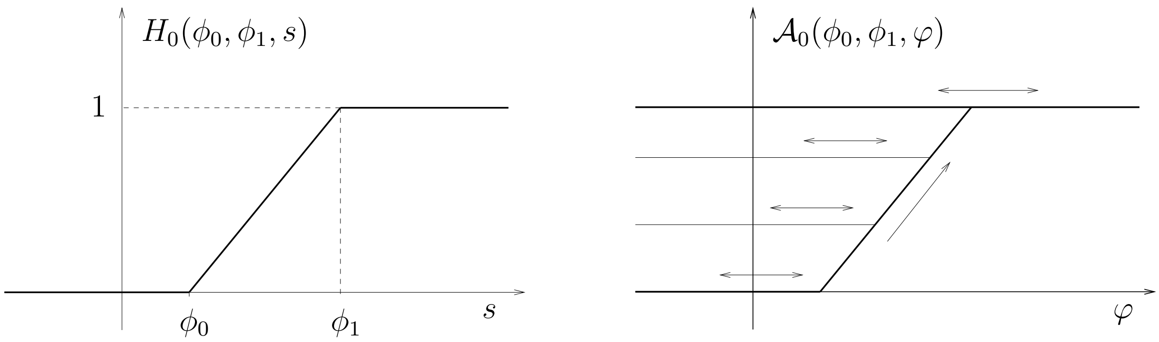


Figure 2: Hysteresis operator $\mathcal{A}$.

holds the protein molecules. It is reasonable to rescale the model from practical point of view. The sensor is developed to detect the presence of a substance whose concentration is very small. Additionally, the thickness of the aptamer layer is also very small. Usually, $\phi \approx 10^{-8}$ and $\sigma \approx 10^{-9}m$. On the other hand, η can assume any value from the interval $[0, 1]$. By this reason, we introduce a scaled concentration $u = \sigma^{-1}\phi$. Note that u can be greater than 1. In order to make the diffusion coefficient being equal to 1, we rescale the time variable multiplying it by α. In the new variables, the problem reads as follows.

$$u_t = \Delta u, \qquad \boldsymbol{x} \in \Omega, \quad t \in [0, T], \tag{1.7}$$

$$t = 0 : \quad u = u^0, \quad \eta = \eta^0, \tag{1.8}$$

$$\partial\Omega \setminus \Gamma : \quad \frac{\partial u}{\partial \nu} = 0, \tag{1.9}$$

$$\Gamma : \quad \eta_t = -\frac{\partial u}{\partial \nu}, \quad \eta = \mathcal{A}(u), \tag{1.10}$$

where $\mathcal{A}(\cdot) = \mathcal{A}_0(a_0, a_1, \cdot)$, $a_0 = \phi_0/\sigma$, $a_1 = \phi_1/\sigma$. We introduce also the function $H(\cdot) = H_0(a_0, a_1, \cdot)$ so that

$$\mathcal{A}(\varphi)(t) = \operatorname*{ess\,sup}_{0 \le \tau \le t} H\big(\varphi(\tau)\big).$$

Problem (1.7)—(1.10) is called *Problem A*.

Remark. It would be more correct to write $\eta = \mathcal{A}(\gamma_0 u)$ in (1.10), where $\gamma_0 : H^1(\Omega) \to H^{1/2}(\Gamma)$ is the trace operator. We omit the symbol γ_0, whenever that does not lead to a confusion. •

1.2 The main result

Denote $\Omega_T = \Omega \times [0, T]$, $\Gamma_T = \Gamma \times [0, T]$. Let ds be the two-dimensional Lebesgue measure.

Definition 1.1 *A pair of functions u, η such that*

$$u \in H^1(\Omega_T), \quad u|_{t=0} = u^0, \quad \eta \in L^\infty(\Gamma_T), \quad \eta_t \in L^2(\Gamma_T)$$

is called a generalized solution to Problem A if

$$\eta(\boldsymbol{x}, t) = \mathcal{A}(u(\boldsymbol{x}, \cdot))(t) \tag{1.11}$$

for almost all $(\boldsymbol{x},t)\in\Gamma_T$*, and the following integral identity*

$$\int_0^T\int_\Omega\big(u_t\psi+\nabla u\cdot\nabla\psi\big)\,d\boldsymbol{x}dt-\int_0^T\int_\Gamma\eta\psi_t\,dsdt+\int_\Gamma\eta^0\psi^0\,ds=0 \tag{1.12}$$

holds for every smooth function ψ *with* $\psi|_{t=T}=0$*. Here* $\psi^0=\psi|_{t=0}$ *and* $\eta^0=\eta|_{t=0}$*.*

The main result of this paper is the following theorem.

Theorem 1.2 *Let* $u^0\in H^1(\Omega)\cap L^\infty(\Omega)$*,* $u^0\geq 0$*, and* η^0 *is a measurable function such that* $\eta^0(\boldsymbol{x})=H\big(u^0(\boldsymbol{x})\big)$ *for* $\boldsymbol{x}\in\Gamma$*. Then there exists a unique generalized solution to Problem A such that*

$$u_t,\Delta u\in L^2(\Omega_T),\quad u_x\in L^\infty(0,T;L^2(\Omega)),$$
$$0\leq u\leq\|u^0\|_{L^\infty(\Omega)},$$
$$\eta_t\in L^2(\Gamma_T),\quad \eta\in H^{1/2}(\Gamma_T).$$

Remark. The condition $\eta^0=H(u^0)$ is not important and can be omitted. It makes a physical sense and, besides that, simplifies some mathematical calculations. •

1.3 Bibliographical remarks

Problems with hysteresis were considered in numerous publications. We refer to the books [1], [2], [3] and [4] for survives in this theory. The common feature of the investigations cited is that the regularizing term $\varepsilon\frac{\partial u}{\partial t}$ is being added to the boundary condition (1.10) to improve the regularity of $u|_\Gamma$ with respect to t. Thus, the boundary condition on Γ looks like that

$$\varepsilon\frac{\partial u}{\partial t}+\eta_t=-\frac{\partial u}{\partial\nu},\quad \eta=\mathcal{A}(u).$$

A technique proposed in this paper allows us to handle the singular case, $\varepsilon=0$.

2 Proof of the main result

2.1 Construction of approximate solutions

Use the following implicit time discretization scheme to approximate the problem. Fix arbitrary $N\in\mathbb{N}$ and set $\tau=T/N$. For every $n\in\{1,2,\dots,N\}$ consider the following problem for u^n:

$$u^n-u^{n-1}=\tau\Delta u^n,\qquad \boldsymbol{x}\in\Omega, \tag{2.1}$$

$$\eta^n-\eta^{n-1}=-\tau\frac{\partial u^n}{\partial\nu},\qquad \boldsymbol{x}\in\Gamma, \tag{2.2}$$

$$\frac{\partial u^n}{\partial\nu}=0,\qquad \boldsymbol{x}\in\partial\Omega\setminus\Gamma. \tag{2.3}$$

where

$$\eta^n(\boldsymbol{x})=\max_{k\in\{0,1,\dots,n\}}H\big(u^k(\boldsymbol{x})\big),\qquad \boldsymbol{x}\in\Gamma. \tag{2.4}$$

Notice that

$$\eta^n(\boldsymbol{x})=\eta^{n-1}(\boldsymbol{x})+\Big(H\big(u^n(\boldsymbol{x})\big)-\eta^{n-1}(\boldsymbol{x})\Big)^+,\qquad \boldsymbol{x}\in\Gamma, \tag{2.5}$$

where $f^+ := \max\{0, f\}$ is the positive part of a function f. The problem (2.1)—(2.4) can be solved by minimization of the following functional in $H^1(\Omega)$:

$$\Phi_n(u) = \int\limits_\Omega \Big(\frac{\tau}{2}\,|\nabla u|^2 + \frac{1}{2}\,|u - u^{n-1}|^2\Big)\,d\boldsymbol{x} + \int\limits_\Gamma F(u, \eta^{n-1})\,ds,$$

where

$$F(u, v) = \int_0^u \big(H(\xi) - v\big)^+\,d\xi.$$

It is not difficult to see that the set of minimizers of the functional Φ_n coincides with the set of solutions to the problem (2.1)–(2.4) for every $n \in \{1, 2, \ldots, N\}$. Since the functional Φ_n is strictly convex, coercive and weakly lower semicontinuous in $H^1(\Omega)$, there exists a unique minimizer $u^n \in H^1(\Omega)$ of Φ_n so that

$$\Phi_n(u^n) = \min_{u \in H^1(\Omega)} \Phi_n(u)$$

for each $n \in \{1, 2, \ldots, N\}$. Some useful estimates can be obtained for the minimizers. The obvious inequality $\Phi_k(u^k) \le \Phi_k(u^{k-1})$ results in

$$\int\limits_\Omega \Big(\frac{\tau}{2}\,|\nabla u^k|^2 + \frac{1}{2}\,|u^k - u^{k-1}|^2\Big)\,d\boldsymbol{x} + \int\limits_\Gamma F(u^k, \eta^{k-1})\,ds \le$$

$$\le \int\limits_\Omega \frac{\tau}{2}\,|\nabla u^{k-1}|^2\,d\boldsymbol{x} + \int\limits_\Gamma F(u^{k-1}, \eta^{k-1})\,ds. \quad (2.6)$$

Note that $F(u^{k-1}(\boldsymbol{x}), \eta^{k-1}(\boldsymbol{x})) = 0$ for almost all $\boldsymbol{x} \in \Gamma$. Really, the obvious inequality $H(u^{k-1}) \le \eta^{k-1}$ and the monotonicity of the function H imply that $H(\xi) - \eta^{k-1}(\boldsymbol{x}) \le H(u^{k-1}(\boldsymbol{x})) - \eta^{k-1}(\boldsymbol{x}) \le 0$ for all $\xi \in [0, u^{k-1}(\boldsymbol{x})]$ and almost all $\boldsymbol{x} \in \Gamma$. This proves the claim. Taking the last result into account and summing up the both sides of inequality (2.6) over k from 1 to n yields

$$\int\limits_\Omega |\nabla u^n|^2\,d\boldsymbol{x} + \tau \sum_{k=1}^n \int\limits_\Omega \Big|\frac{u^k - u^{k-1}}{\tau}\Big|^2\,d\boldsymbol{x} \le \int\limits_\Omega |\nabla u^0|^2\,d\boldsymbol{x}. \quad (2.7)$$

Relations (2.7) and (2.1) imply

$$\tau \sum_{k=1}^n \int\limits_\Omega |\Delta u^k|^2\,d\boldsymbol{x} \le \int\limits_\Omega |\nabla u^0|^2\,d\boldsymbol{x}. \quad (2.8)$$

The following lemma proves an auxiliary result that is surely well known an can be found in the literature.

Lemma 2.1 *Let $f : \mathbb{R} \to \mathbb{R}$ be a C^1 function such that f' is non-decreasing. Then*

$$f(\alpha) - f(\beta) \le f'(\alpha)(\alpha - \beta)$$

for all $\alpha, \beta \in \mathbb{R}$.

$\triangleright$ Really, if $\alpha > \beta$, then $f(\alpha) - f(\beta) = f'(\xi_0)(\alpha - \beta) \le f'(\alpha)(\alpha - \beta)$, where $\xi_0 \in [\beta, \alpha]$. If $\alpha < \beta$, then $f(\beta) - f(\alpha) = f'(\xi_0)(\beta - \alpha) \ge f'(\alpha)(\beta - \alpha)$, where $\xi_0 \in [\alpha, \beta]$. $\triangleleft$

Lemma 2.2 *The following inequality*

$$0 \le u^n(\boldsymbol{x}) \le \operatorname*{ess\,sup}_{\boldsymbol{x}\in\Omega} u^0(\boldsymbol{x}).$$

holds for all $n = 1, 2, \dots, N$ *and for almost all* $\boldsymbol{x} \in \Omega$.

$\triangleright$ Denote $b = \operatorname*{ess\,sup}_{\boldsymbol{x}\in\Omega} u^0(\boldsymbol{x})$ and introduce the following function

$$f(\xi) = \begin{cases} \xi^2, & \xi \le 0, \\ 0, & 0 \le \xi \le b, \\ (\xi - b)^2, & \xi \ge b. \end{cases}$$

It is not difficult to see that this function satisfies the conditions of Lemma 2.1. Multiply (2.1) by $f'(u^n)$ and integrate over Ω. This yields

$$\int\limits_{\Omega} \Big(f'(u^n)\,\frac{u^n - u^{n-1}}{\tau} + f''(u^n)|\nabla u^n|^2 \Big)\, d\boldsymbol{x} =$$

$$= \int\limits_{\Gamma} \frac{\partial u^n}{\partial \nu} f'(u^n)\, ds = - \int\limits_{\Gamma} \frac{\eta^n - \eta^{n-1}}{\tau}\, f'(u^n)\, ds \le 0, \quad (2.9)$$

because the function $(\eta^n - \eta^{n-1})f'(u^n)$ is nonnegative on Γ. The last claim is true due to the following arguments. If $u^n(\boldsymbol{x}) \ge 0$, then $f'(u^n(\boldsymbol{x})) \ge 0$, which implies that $\big(\eta^n(\boldsymbol{x}) - \eta^{n-1}(\boldsymbol{x})\big)\, f'(u^n(\boldsymbol{x})) \ge 0$ because $\eta^n \ge \eta^{n-1}$. If $u^n(\boldsymbol{x}) \le 0$, then $\eta^n(\boldsymbol{x}) = \eta^{n-1}(\boldsymbol{x})$ because u^0 is nonnegative.

Due to (2.9), Lemma 2.1 and convexity of the function f, the following is true

$$\int\limits_{\Omega} f(u^n)\, d\boldsymbol{x} \le \int\limits_{\Omega} f(u^{n-1})\, d\boldsymbol{x}.$$

Taking into account that $f(u^0) = 0$ implies that $f(u^n) = 0$. This relation proves the lemma. $\triangleleft$

Denote

$$\zeta^n(\boldsymbol{x}) = \max_{k\in\{0,1,\dots,n\}} H\big(u^k(\boldsymbol{x})\big), \qquad \boldsymbol{x} \in \Omega. \quad (2.10)$$

The equivalent definition of this function reads as

$$\zeta^n(\boldsymbol{x}) = \zeta^{n-1}(\boldsymbol{x}) + \Big(H\big(u^n(\boldsymbol{x})\big) - \zeta^{n-1}(\boldsymbol{x}) \Big)^+, \qquad \boldsymbol{x} \in \Omega. \quad (2.11)$$

It is obvious that $\zeta^n \in H^1(\Omega)$ and

$$\eta^n = \gamma_0 \zeta^n. \quad (2.12)$$

The following lemma gives some uniform estimates for ζ^n and η^n.

Lemma 2.3 *For all* $n = 1, 2, \dots, N$*, the following is true*

$$\int\limits_{\Omega} |\nabla \zeta^n|^2\, d\boldsymbol{x} \le c_0^2 \int\limits_{\Omega} |\nabla u^0|^2\, d\boldsymbol{x}, \quad (2.13)$$

$$\tau \sum_{k=1}^{n} \int\limits_{\Omega} \Big(\frac{\zeta^k - \zeta^{k-1}}{\tau} \Big)^2\, d\boldsymbol{x} \le \frac{c_0^2}{2} \int\limits_{\Omega} |\nabla u^0|^2\, d\boldsymbol{x}, \quad (2.14)$$

$$\tau \sum_{k=1}^{n} \int_{\Gamma} \Big(\frac{\eta^k - \eta^{k-1}}{\tau}\Big)^2 \, ds \le \frac{c_0}{2} \int_{\Omega} |\nabla u^0|^2 \, d\boldsymbol{x}, \tag{2.15}$$

where $c_0 = \max_{s\in\mathbb{R}} \big(dH(s)/ds\big)$.

$\triangleright$ Denote

$$\xi^n(\boldsymbol{x}) = \max_{k\in\{0,1,\dots,n\}} u^k(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega.$$

It is not difficult to see that $\zeta^n = H(\xi^n)$. Denote the set in Ω where $u^n \ge \xi^{n-1}$ by G^n. Multiplying (2.1) by $\xi^n - \xi^{n-1}$ yields

$$\int_{\Omega} \Big((u^n - u^{n-1})(\xi^n - \xi^{n-1}) + \tau \nabla u^n \cdot \nabla(\xi^n - \xi^{n-1}) \Big) \, d\boldsymbol{x} + \int_{\Gamma} (\eta^n - \eta^{n-1})(\xi^n - \xi^{n-1}) \, ds = 0.$$

Note that $(u^n - u^{n-1})(\xi^n - \xi^{n-1}) \ge (\xi^n - \xi^{n-1})^2$ almost everywhere in Ω. Really, if $\boldsymbol{x} \in G^n$, then $\xi^n(\boldsymbol{x}) = u^n(\boldsymbol{x})$ and $u^n(\boldsymbol{x}) - u^{n-1}(\boldsymbol{x}) \ge u^n(\boldsymbol{x}) - \xi^{n-1}(\boldsymbol{x}) = \xi^n(\boldsymbol{x}) - \xi^{n-1}(\boldsymbol{x})$. If $\boldsymbol{x} \notin G^n$, then $\xi^n(\boldsymbol{x}) = \xi^{n-1}(\boldsymbol{x})$ and $(u^n(\boldsymbol{x}) - u^{n-1}(\boldsymbol{x}))(\xi^n(\boldsymbol{x}) - \xi^{n-1}(\boldsymbol{x})) = (\xi^n(\boldsymbol{x}) - \xi^{n-1}(\boldsymbol{x}))^2 = 0$. Thus,

$$\int_{\Omega} (\xi^n - \xi^{n-1})^2 \, d\boldsymbol{x} + \int_{\Gamma} (\eta^n - \eta^{n-1})(\xi^n - \xi^{n-1}) \, ds + \tau \int_{\Omega} \nabla u^n \cdot \nabla(\xi^n - \xi^{n-1}) \, d\boldsymbol{x} \le 0. \tag{2.16}$$

It is clear that $\nabla(\xi^n - \xi^{n-1}) = 0$ almost everywhere in $\Omega \setminus G^n$. On the other hand, $u^n = \xi^n$ and $\nabla u^n = \nabla \xi^n$ almost everywhere in G^n. Therefore,

$$\int_{\Omega} \nabla u^n \cdot \nabla(\xi^n - \xi^{n-1}) \, d\boldsymbol{x} = \int_{G^n} \nabla u^n \cdot \nabla(\xi^n - \xi^{n-1}) \, d\boldsymbol{x} =$$
$$= \int_{G^n} \nabla \xi^n \cdot \nabla(\xi^n - \xi^{n-1}) \, d\boldsymbol{x} = \int_{\Omega} \nabla \xi^n \cdot \nabla(\xi^n - \xi^{n-1}) \, d\boldsymbol{x} =$$
$$= \frac{1}{2} \int_{\Omega} |\nabla \xi^n|^2 \, d\boldsymbol{x} - \frac{1}{2} \int_{\Omega} |\nabla \xi^{n-1}|^2 \, d\boldsymbol{x} + \frac{1}{2} \int_{\Omega} |\nabla \xi^n - \nabla \xi^{n-1}|^2 \, d\boldsymbol{x}.$$

This relation together with (2.16) gives

$$\frac{2}{\tau} \sum_{k=1}^{n} \int_{\Omega} (\xi^k - \xi^{k-1})^2 \, d\boldsymbol{x} + \frac{2}{\tau} \sum_{k=1}^{n} \int_{\Gamma} (\eta^k - \eta^{k-1})(\xi^k - \xi^{k-1}) \, ds + \int_{\Omega} |\nabla \xi^n|^2 \, d\boldsymbol{x} \le \int_{\Omega} |\nabla u^0|^2 \, d\boldsymbol{x}.$$

Note that $\zeta^k - \zeta^{k-1} = H(\xi^k) - H(\xi^{k-1}) \le c_0(\xi^k - \xi^{k-1})$, where $c_0 = \max_{s\in\mathbb{R}} \big(dH(s)/ds\big) > 0$. Therefore, multiplying the last estimate by c_0^2 gives

$$\frac{2}{\tau} \sum_{k=1}^{n} \int_{\Omega} (\zeta^k - \zeta^{k-1})^2 \, d\boldsymbol{x} + \frac{2c_0}{\tau} \sum_{k=1}^{n} \int_{\Gamma} (\eta^k - \eta^{k-1})^2 \, ds + c_0^2 \int_{\Omega} |\nabla \xi^n|^2 \, d\boldsymbol{x} \le c_0^2 \int_{\Omega} |\nabla u^0|^2 \, d\boldsymbol{x}.$$

The assertion of the lemma follows immediately from this inequality. $\triangleleft$

2.2 Passage to the limit

For every $N \in \mathbb{N}$, let u_N, η_N, and ζ_N be piecewise linear time interpolations of $\{u^n\}$, $\{\eta^n\}$ and $\{\zeta^n\}$, respectively; $\overline{u}_N$, $\overline{\eta}_N$, and $\overline{\zeta}_N$ piecewise constant time interpolations of these functions. Remember that piecewise linear and piecewise constant time interpolations of a function $v(x,t)$ are given by

$$v_N(\boldsymbol{x},t) = v^n(\boldsymbol{x})\Big(1 - n + \frac{t}{\tau}\Big) + v^{n-1}(\boldsymbol{x})\Big(n - \frac{t}{\tau}\Big), \qquad \text{if} \quad t \in [(n-1)\tau, n\tau],$$

and

$$\overline{v}_N(\boldsymbol{x},t) = v^n(\boldsymbol{x}), \qquad \text{if} \quad t \in ((n-1)\tau, n\tau],$$

respectively.

Lemma 2.4

$$(u_N - \overline{u}_N) \to 0, \quad (\zeta_N - \overline{\zeta}_N) \to 0 \qquad \text{in} \quad L^2(\Omega_T),$$
$$(\eta_N - \overline{\eta}_N) \to 0 \qquad \text{in} \quad L^2(\Gamma_T)$$

as $N \to \infty$.

$\triangleright$ Due to (2.7),

$$\int\limits_0^T \|u_N(t) - \overline{u}_N(t)\|^2_{L^2(\Omega)}\, dt = \sum_{n=1}^N \|u^n - u^{n-1}\|^2_{L^2(\Omega)} \int\limits_{(n-1)\tau}^{n\tau} \Big(\frac{t}{\tau} - n\Big)^2 dt =$$
$$= \frac{\tau}{3} \sum_{n=1}^N \|u^n - u^{n-1}\|^2_{L^2(\Omega)} \le \frac{\tau^2}{3} \|\nabla u^0\|^2_{L^2(\Omega)}.$$

Since $\tau = 1/N$, the first assertion is proved. The other two claims can be proved with the same arguments using estimates (2.14) and (2.15). $\triangleleft$

Estimates (2.7),(2.8),(2.13),(2.14), and (2.15) imply

$$\Big\|\frac{\partial u_N}{\partial t}\Big\|^2_{L^2(\Omega_T)} + \|\nabla \overline{u}_N\|^2_{L^\infty(0,T;L^2(\Omega))} \le \|\nabla u^0\|^2_{L^2(\Omega)},$$
$$\|\nabla u_N\|_{L^\infty(0,T;L^2(\Omega))} \le \|\nabla u^0\|_{L^2(\Omega)}, \qquad \|\Delta \overline{u}_N\|_{L^2(\Omega_T)} \le \|\nabla u^0\|_{L^2(\Omega)},$$
$$\|\nabla \overline{\zeta}_N\|_{L^\infty(0,T;L^2(\Omega))} \le c_0 \|\nabla u^0\|_{L^2(\Omega)}, \qquad \|\nabla \zeta_N\|_{L^\infty(0,T;L^2(\Omega))} \le c_0 \|\nabla u^0\|_{L^2(\Omega)},$$
$$\Big\|\frac{\partial \zeta_N}{\partial t}\Big\|_{L^2(\Omega_T)} \le \frac{c_0}{\sqrt{2}} \|\nabla u^0\|_{L^2(\Omega)}, \qquad \Big\|\frac{\partial \eta_N}{\partial t}\Big\|_{L^2(\Gamma_T)} \le \sqrt{\frac{c_0}{2}} \|\nabla u^0\|_{L^2(\Omega)}.$$

These estimates along with (2.1)–(2.4) yield

$$\frac{\partial u_N}{\partial t} = \Delta \overline{u}_N \qquad \text{in} \quad L^2(\Omega_T), \tag{2.17}$$
$$\frac{\partial \eta_N}{\partial t} = -\frac{\partial \overline{u}_N}{\partial \nu} \qquad \text{in} \quad L^2(0,T;H^{-1/2}(\Gamma)), \tag{2.18}$$
$$\frac{\partial \overline{u}_N}{\partial \nu} = 0 \qquad \text{in} \quad L^2(0,T;H^{-1/2}(\partial\Omega \setminus \Gamma)), \tag{2.19}$$
$$\overline{\eta}_N(\boldsymbol{x},t) = \mathcal{A}(\overline{u}_N(\boldsymbol{x},\cdot))(t) \qquad \text{for a.a.} \quad (\boldsymbol{x},t) \in \Gamma_T, \tag{2.20}$$
$$\overline{\zeta}_N(\boldsymbol{x},t) = \mathcal{A}(\overline{u}_N(\boldsymbol{x},\cdot))(t) \qquad \text{for a.a.} \quad (\boldsymbol{x},t) \in \Omega_T. \tag{2.21}$$

Besides that, (2.12) implies

$$\overline{\eta}_N = \gamma_0 \overline{\zeta}_N \qquad \text{in} \quad L^\infty(0,T;H^{1/2}(\Gamma)). \tag{2.22}$$

Thanks to the estimates obtained above and to Lemma 2.4, there exist a sequence $N_m \to \infty$ and functions u, η and ζ such that

$$\begin{aligned}
&u_{N_m} \to u && * \text{ weakly in} \quad H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)),\\
&\overline{u}_{N_m} \to u && * \text{ weakly in} \quad L^\infty(0,T;H^1(\Omega)),\\
&\zeta_{N_m} \to \zeta && * \text{ weakly in} \quad H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)),\\
&\overline{\zeta}_{N_m} \to \zeta && * \text{ weakly in} \quad L^\infty(0,T;H^1(\Omega)),\\
&\eta_{N_m} \to \eta && \text{weakly in} \quad H^1(0,T;L^2(\Gamma)),\\
&\overline{\eta}_{N_m} \to \eta && * \text{ weakly in} \quad L^\infty(0,T;H^{1/2}(\Gamma)),
\end{aligned}$$

As a consequence, we have

$$\begin{aligned}
&u \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \qquad \Delta u \in L^2(\Omega_T),\\
&\zeta \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)),\\
&\eta \in H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{1/2}(\Gamma)),
\end{aligned}$$

Moreover, due to Lemma 2.2, the functions u, η and ζ are bounded and

$$0 \le u(\boldsymbol{x},t) \le \operatorname*{ess\,sup}_{\boldsymbol{x}\in\Omega} u^0(\boldsymbol{x}).$$

The passage to the limit in (2.17)–(2.19), and (2.22) with respect to subsequences yields

$$\frac{\partial u}{\partial t} = \Delta u \qquad \text{in} \quad L^2(\Omega_T), \tag{2.23}$$

$$\frac{\partial \eta}{\partial t} = -\frac{\partial u}{\partial \nu} \qquad \text{in} \quad L^2(0,T;H^{-1/2}(\Gamma)), \tag{2.24}$$

$$\frac{\partial u}{\partial \nu} = 0 \qquad \text{in} \quad L^2(0,T;H^{-1/2}(\partial\Omega \setminus \Gamma)), \tag{2.25}$$

$$\eta = \gamma_0 \zeta \qquad \text{in} \quad L^\infty(0,T;H^{1/2}(\Gamma)). \tag{2.26}$$

In order to complete the proof of the solvability of Problem A, we have to establish (1.11). First, we prove that

$$\zeta(\boldsymbol{x},t) = \mathcal{A}(u(\boldsymbol{x},\cdot))(t) \qquad \text{for almost all} \quad (\boldsymbol{x},t) \in \Omega_T. \tag{2.27}$$

The prove uses arguments that are similar to those from [2, IX.1]. Namely, standard results yield the following embeddings for every $s \in (0,1/2)$:

$$H^1(\Omega_T) \subset H^s(\Omega;H^{1-s}(0,T)) \subset L^2(\Omega;C^\alpha[0,T]),$$

where $\alpha < 1/2 - s$. The last embedding is compact. Therefore, $u_{N_m} \to u$ in $L^2(\Omega;C^\alpha[0,T])$ and $u_{N_m}(\boldsymbol{x},\cdot) \to u(\boldsymbol{x},\cdot)$ in $C^\alpha[0,T]$ for almost all $\boldsymbol{x} \in \Omega$. Fix an arbitrary $t \in [0,T]$. For every $N_m \in \mathbb{N}$, there exist $n \in \{1,\dots,N_m\}$ such that $t \in ((n-1)\tau, n\tau]$. Thus,

$$\begin{aligned}
\mathcal{A}(\overline{u}_{N_m}(\boldsymbol{x},\cdot))(t) = \operatorname*{ess\,sup}_{s\in[0,t]} H(\overline{u}_{N_m}(\boldsymbol{x},s)) = \operatorname*{ess\,sup}_{s\in[0,n\tau]} H(\overline{u}_{N_m}(\boldsymbol{x},s)) = \\
= \max_{s\in[0,n\tau]} H(u_{N_m}(\boldsymbol{x},s)) = \max_{s\in[0,t]} H(u_{N_m}(\boldsymbol{x},s)) + R(\tau,u_{N_m},t),
\end{aligned}$$

where $|R(\tau, u_{N_m}, t)| \le C\,\tau^\alpha$ with a constant C which is independent of N_m and t. The passage to the limit in (2.21) gives (2.27).

Due to (2.26) and (2.27), it remains to prove only that

$$\gamma_0 \mathcal{A}(u)(t) = \mathcal{A}(\gamma_0 u)(t) \qquad \text{for almost all} \quad t \in [0, T], \tag{2.28}$$

where u is the limit of $\{u_{N_m}\}$. To do that, some regularity properties of the function u should be established.

Lemma 2.5 *For every $\delta > 0$, there exists $\beta \in (0,1)$ such that $u \in C^{\alpha,\alpha/2}(\overline{Q})$, where Q is an arbitrary subdomain of Ω_T such that $\overline{Q} \subset \overline{\Omega_T}$ and* $\operatorname{dist}(Q, \{(\boldsymbol{x}, t) \in \mathbb{R}^{3+1} \,|\, t = 0\}) > \delta$.

$\triangleright$ Take an arbitrary number $k \in \mathbb{R}$ and multiply (2.23) by $(u-k)^+$. Integration of the product over Ω gives

$$\frac{1}{2}\frac{d}{dt}\int\limits_\Omega \left((u-k)^+\right)^2 d\boldsymbol{x} + \int\limits_\Omega \left|\nabla (u-k)^+\right|^2 d\boldsymbol{x} = -\int\limits_\Gamma \eta_t (u-k)^+\, ds \le 0,$$

because η does not decrease in t. The assertion of the lemma follows now from Theorem 1.7 of [6]. $\triangleleft$

For every $\delta > 0$, introduce the following operator

$$\mathcal{A}_\delta(v)(t) = \begin{cases} 0, & t < \delta, \\ \operatorname*{ess\,sup}\limits_{\delta \le s \le t} H(v(s)), & t \ge \delta, \end{cases}$$

where $v \in L^\infty(0,T)$. Since u is continuous in $\overline{\Omega} \times [\delta, T]$, the relation holds

$$\gamma_0 \mathcal{A}_\delta(u)(t) = \mathcal{A}_\delta(\gamma_0 u)(t) \qquad \text{for all} \quad t \in [0, T]. \tag{2.29}$$

Note that $\mathcal{A}(v)(t) = \|v\|_{L^\infty(0,t)}$ for any nonnegative function $v \in L^\infty(0,T)$, and $\mathcal{A}_\delta(v)(t) = \|\chi_\delta v\|_{L^\infty(0,t)}$, where $\chi_\delta : \mathbb{R} \to \{0,1\}$ is the characteristic function of the interval (δ, T). It is clear that $\mathcal{A}(v)(t) \ge \mathcal{A}_\delta(v)(t)$. On the other hand, $\mathcal{A}(v)(t) \le \liminf\limits_{\delta \to 0} \mathcal{A}_\delta(v)(t)$ due to the $*$ weak semi-continuity of the norm in L^∞. The two last inequalities provide

$$\mathcal{A}(v)(t) = \lim_{\delta \to 0} \mathcal{A}_\delta(v)(t)$$

for almost all $t \in [0,T]$ and for every nonnegative function $v \in L^\infty(0,T)$. Passage to the limit in (2.29) as $\delta \to 0$ gives (2.28).

The solvability of the Problem A is proved.

2.3 Uniqueness of the solution

Let $\{u_k, \eta_k\}$, $k = 1,2$, be two solutions of Problem A. Denote $\tilde{u} = u_1 - u_2$, $\tilde{\eta} = \eta_1 - \eta_2$. Due to the Hilpert's inequality (see [2, III.2])

$$\frac{d\tilde{\eta}^+(\boldsymbol{x},\cdot)}{dt} \le \frac{d\tilde{\eta}(\boldsymbol{x},\cdot)}{dt}\, q(\boldsymbol{x},\cdot), \qquad \text{a.e. in} \quad (0,T) \tag{2.30}$$

for almost all $\boldsymbol{x} \in \Gamma$ and for every measurable function $q(\boldsymbol{x},\cdot) \in H_e(\tilde{u}(\boldsymbol{x},\cdot))$, where

$$H_e(s) = \begin{cases} 0, & s < 0, \\ [0,1], & s = 0, \\ 1, & s > 0. \end{cases}$$

Multiply (1.7) by $q_m(\boldsymbol{x}, t) = H_e^m(\tilde{u}(\boldsymbol{x}, t))$, where

$$H_e^m(s) = \begin{cases} 0, & s < 0, \\ ms, & 0 \le s \le 1/m, \\ 1, & s > 1/m. \end{cases}$$

The inequality

$$\int_\Omega \nabla \tilde{u} \cdot \nabla q_m \, d\boldsymbol{x} = \int_\Omega (H_e^m)'(\tilde{u}) \, |\nabla \tilde{u}|^2 \, d\boldsymbol{x} \ge 0,$$

implies

$$\int_\Omega \frac{\partial \tilde{u}}{\partial t} H_e^m(\tilde{u}) \, d\boldsymbol{x} + \int_\Gamma \frac{\partial \tilde{\eta}}{\partial t} H_e^m(\tilde{u}) \, ds \le 0 \qquad \text{a.e. in} \quad (0, T).$$

Passage to the limit as $m \to 0$ gives

$$\int_\Omega \frac{\partial \tilde{u}^+}{\partial t} \, d\boldsymbol{x} + \int_\Gamma \frac{\partial \tilde{\eta}}{\partial t} q \, ds \le 0 \qquad \text{a.e. in} \quad (0, T),$$

where $q \in H_e(\tilde{u})$ is a function such that $H_e^m(\tilde{u}) \to q$ almost everywhere in Γ_T. Therefore, inequality (2.30) implies

$$\frac{d}{dt}\Big(\int_\Omega \tilde{u}^+ \, d\boldsymbol{x} + \int_\Gamma \tilde{\eta}^+ \, ds \Big) \le 0.$$

This means that $\tilde{u}^+ = 0$ and $\tilde{\eta}^+ = 0$. Interchanging indices 1 and 2 in the definition of $\tilde{u}$ and $\tilde{\eta}$, we conclude that $\tilde{u} = 0$ and $\tilde{\eta} = 0$. The theorem is proved.

2.4 Numerical simulation

First, consider a two-dimensional case, where the solution is assumed being independent on the x_2 variable. Set $a_0 = 0$ and $a_1 = 0.1$ in the definition of the function H. The initial concentration u_0 is of the form

$$u_0(x_1, x_2) = \begin{cases} 10, \text{ if } (x_1 - 0.2)^2 + (x_2 - 0.2)^2 < 0.12^2; \\ 15, \text{ if } (x_1 - 0.7)^2 + (x_2 - 0.2)^2 < 0.1^2; \\ 0, \text{ otherwise.} \end{cases}$$

Simulation results are shown in figure 3. The concentration $u|_\Gamma$ grows at the beginning, see graphs $a')$ and $b')$. Then, $u|_\Gamma$ goes down because the substance is being spread out over the whole volume of the wet cell, see graphs $c')$, $d')$, and $e')$. The surface concentration η grows monotonically and shows a saturation at the value equal to 1, see $a)$ - $e)$. Note that $u|_\Gamma$ grows drastically at the regions where η archives the saturation because the flux through Γ stops at such regions, compare graphs $b)$ and $b')$.

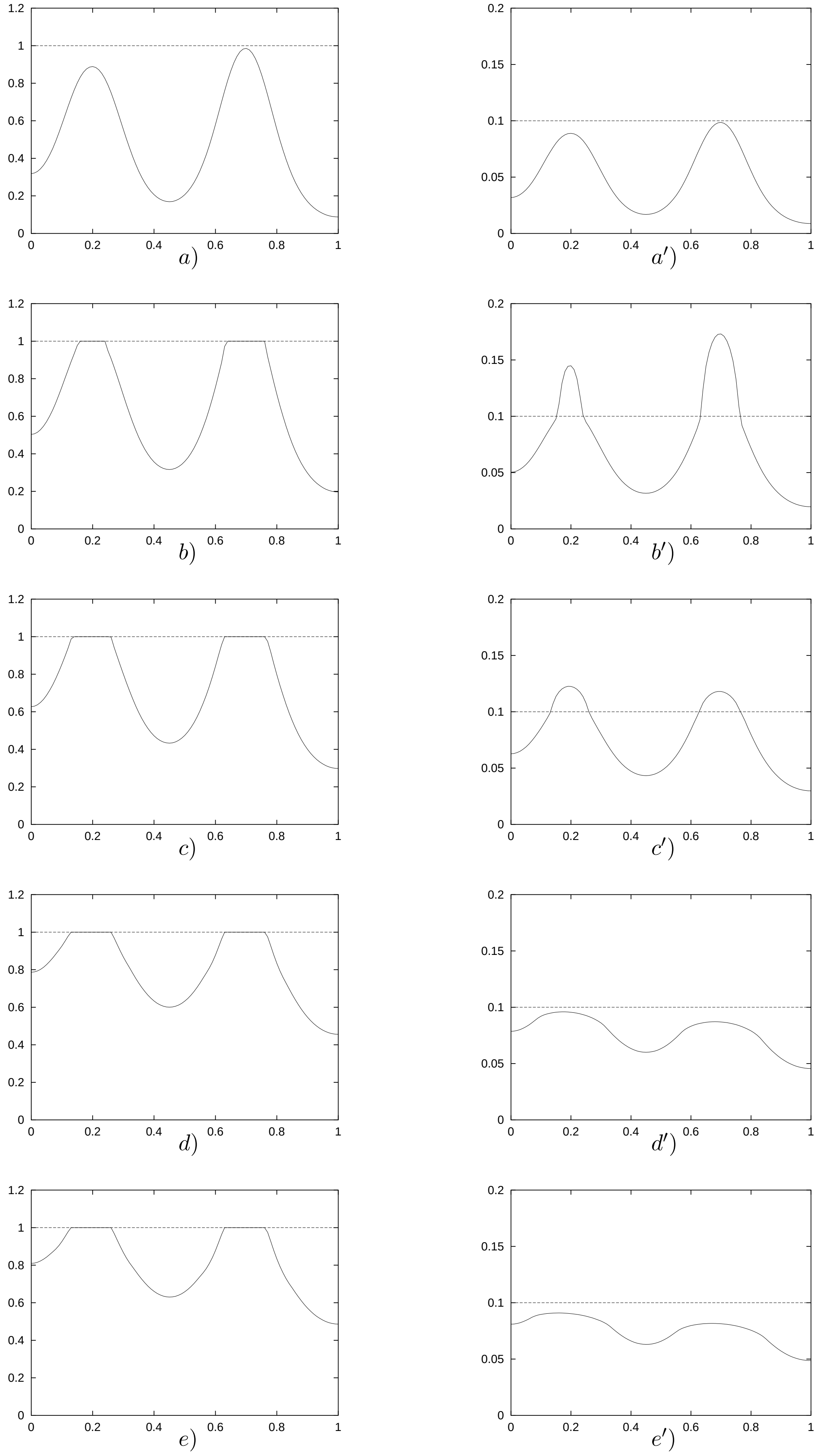
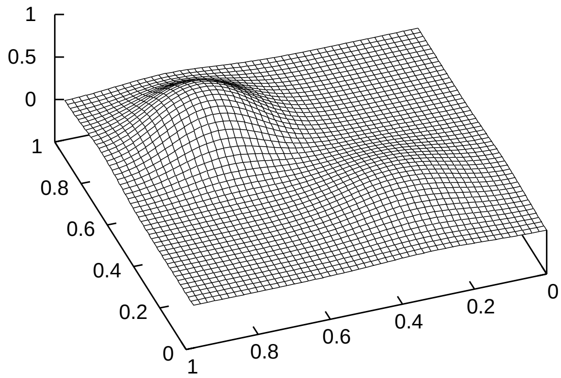


Figure 3. Time development of the concentration u (to the right) and the surface concentration η (to the left) at the bottom Γ for several time instances.

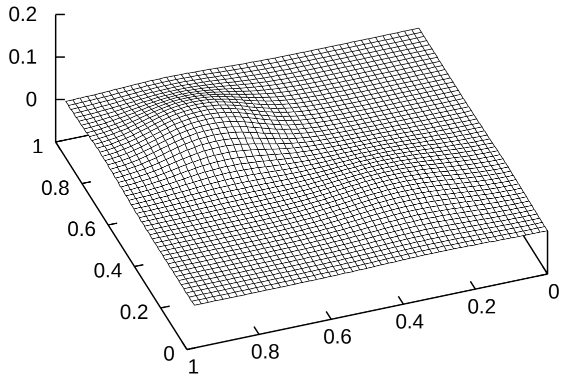
Now consider a three dimensional case. The parameters $a_0 = 0$ and $a_1 = 0.1$ in the definition of the function H are the same as in the two dimensional case. The initial concentration u_0 is now of the form

$$u_0(x_1, x_2, x_3) = \begin{cases} 13, \text{ if } (x_1 - 0.3)^2 + (x_2 - 0.3)^2 + (x_3 - 0.4)^2 < 0.2^2; \\ 12, \text{ if } (x_1 - 0.7)^2 + (x_2 - 0.7)^2 + (x_3 - 0.3)^2 < 0.2^2; \\ 0, \text{ otherwise.} \end{cases}$$

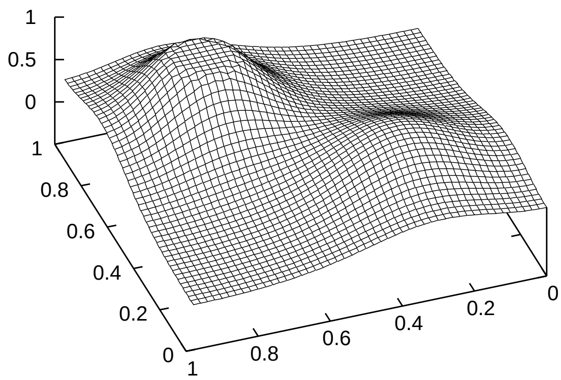
Figure 4. shows simulation results. The qualitative behavior of $u|_\Gamma$ and η is similar to that in the two dimensional case: $u|_\Gamma$ grows at the beginning and then goes down. The surface concentration η grows monotonically and archives a saturation at 1. The grows of $u|_\Gamma$ is very quick in the regions where η archives the saturation.



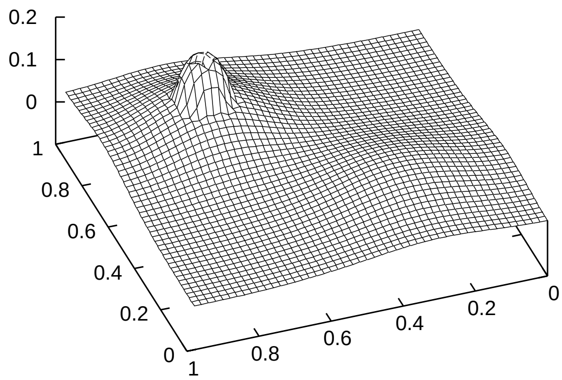
$a)$



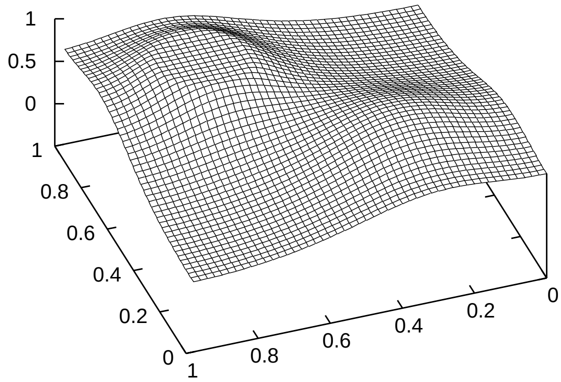
$a')$



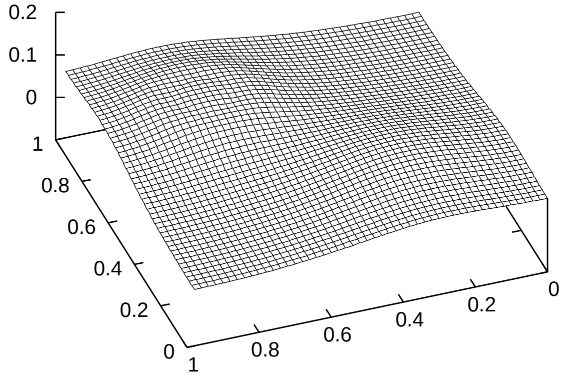
$b)$



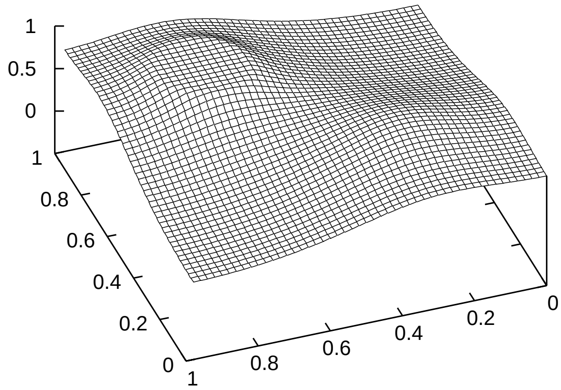
$b')$



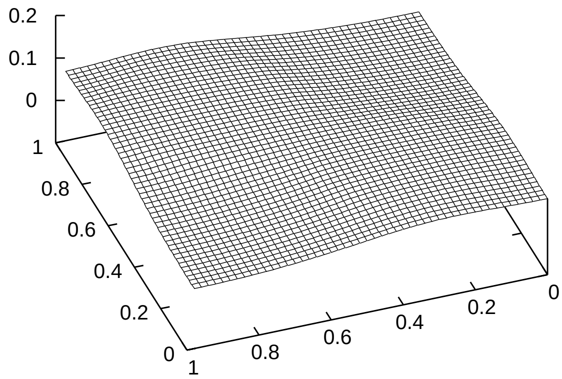
$c)$



$c')$



$d)$



$d')$

Figure 4. Time development of the concentration u (to the right) and the surface concentration η (to the left) at the bottom Γ for several time instances.

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