Transport equation with boundary conditions of hysteresis type

T. G. Amler[1,*,†,‡], N. D. Botkin[1], K.-H. Hoffmann[1], A. M. Meirmanov[2] and V. N. Starovoitov[3]

[1] *Department of Mathematics, Technische Universität München, 85748 Garching bei München, Germany*
[2] *The State University of Belgorod, Russia*
[3] *Lavrentyev Institute of Hydrodynamics, Siberian Branch of RAS, Russian Federation*

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SUMMARY

This paper is an advanced extension of the work reported in (*Nonlinear Anal.* 2005; **63**:1467–1473). A transport equation that describes the propagation of a substance in a moving fluid or gas is considered. The equation contains the transient, convection, and diffusion terms. The problem is formulated in a bounded domain provided with an inlet and an outlet for the fluid or gas flow. The crucial point of the problem setting is a hysteresis-type condition posed on an active part of the boundary. This condition reflects the nondecreasing accumulation with saturation of the transported substance at each point of the active boundary part. We prove the existence and uniqueness of solutions to this problem, study the regularity properties of solutions, and perform numerical simulations that clarify the behavior of the model. Comparing with the results of (*Nonlinear Anal.* 2005; **63**:1467–1473), the advancement of this work consists in accounting for the motion of the fluid or gas and posing inlet and outlet boundary conditions.

KEY WORDS: biosensor; protein detection; hysteresis; boundary value problem; transport equation

1. INTRODUCTION

The objective of this paper is to extend the results obtained in [1]. Remember that the problem under consideration is motivated by the development of biosensors that serve for the quantitative detection of proteins in solutions. An important part of such sensors is a wet cell, say a tiny box, provided with an inlet and an outlet for the solution containing a protein to be detected.

*Correspondence to: T. G. Amler, Department of Mathematics, Technische Universität München, 85748 Garching bei München, Germany.
†E-mail: thomas.amler@mytum.de
‡Chair of Mathematical Modelling.

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Special molecules called aptamers are immobilized at 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. This paper extends the model considered in [1] for the propagation of the protein in the wet cell and its adhering to the aptamer. It is assumed now that the propagation of the injected protein is governed by a transport equation that contains the transition, convection, and diffusion terms. The problem is considered in a bounded domain provided with an inlet and an outlet for the fluid. As in [1], a boundary condition of hysteresis type is posed at the bottom of the wet cell. This condition provides the monotone growth with saturation of the surface concentration of the deposited protein. The monotonicity reflects the nondetachment of already adhered protein molecules, whereas the saturation corresponds to the exhaustion of free aptamer molecules.

We prove the existence and the uniqueness of solutions to this problem, study their regularity, and present numerical simulations.

1.1. Model setting

Let $\Omega=(0,1)^3$ be the open unit cube in $\mathbb{R}^3$ (the wet cell); $\partial\Omega$ the boundary of Ω; $\Gamma=\{\mathbf{x}\in\partial\Omega|x_3=0\}$ an active part of $\partial\Omega$ that can absorb the protein; $\Gamma^{\mathrm{in}}\subset\partial\Omega$ and $\Gamma^{\mathrm{out}}\subset\partial\Omega$ are the inlet and outlet areas for the solution containing the protein, respectively.

Let ϕ be the volume fraction of the protein (is of the order of 10^{-9}), ρ_{p} its proper density, and $\mathbf{V}$ the velocity of the fluid. Then the mass conservation law reads

$$\frac{\partial(\rho_p\phi)}{\partial t}=-\operatorname{div}\mathbf{j}\quad \text{with } \mathbf{j}=-\alpha\nabla(\rho_{\mathrm{p}}\phi)+(\rho_{\mathrm{p}}\phi)\mathbf{V} \tag{1}$$

where α is the diffusion coefficient. Assume (see Figure 1) that the protein molecules adhered to the aptamer are small roods of the height $\delta(\approx 10^{-8}\,\mathrm{m})$ immobilized in the layer

$$\Gamma_\delta=\{\mathbf{x}\in\mathbb{R}^3|-\delta\leqslant x_3\leqslant 0,\ (x_1,x_2,0)\in\Gamma\}$$

Let $\bar{\phi}$ be the volume fraction of the protein in Γ_δ, and $\phi_{\max}$ its maximal value ($\phi_{\max}\approx 0.1$). Define the surface density η of the protein as

$$\eta=\frac{1}{\delta\phi_{\max}}\int_{-\delta}^{0}\bar{\phi}\,\mathrm{d}x_3$$

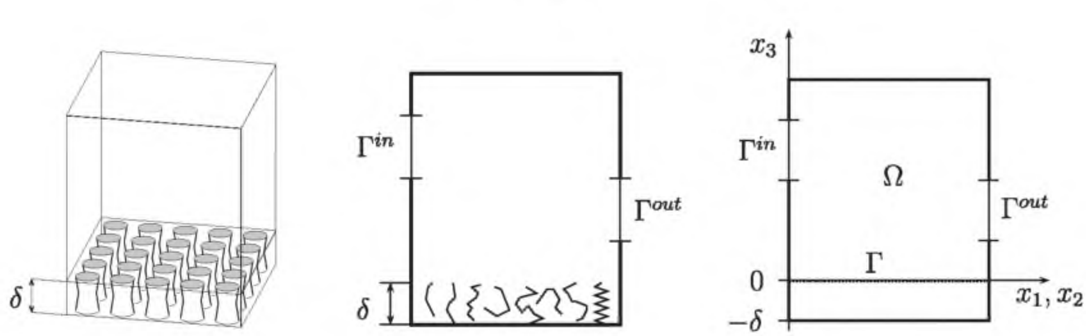

Figure 1. The adhered protein molecules in the layer Γ_δ.

and scale the volume fraction ϕ as follows:

$$u = \frac{1}{\delta\phi_{\max}}\phi \tag{2}$$

Note that the mass of the protein in Γ_δ per surface unit is given by the formula:

$$\mu = \rho_p \int_{-\delta}^{0} \bar{\phi}\,\mathrm{d}x_3 = (\delta\phi_{\max})\rho_p \eta \tag{3}$$

On the other hand, taking into account that the components j_1 and j_2 of $\mathbf{j}$ disappear in Γ_δ because the protein molecules are immediately immobilized after adhering to the aptamer, the mass conservation law says:

$$\frac{\partial \mu}{\partial t} = \mathbf{j}\cdot\mathbf{v} \quad \text{on } \Gamma \tag{4}$$

Combining (4), (3), (2), and (1) yields:

$$\frac{\partial \eta}{\partial t} = -\alpha \nabla u \cdot \mathbf{v} \quad \text{on } \Gamma \tag{5}$$

whenever $\mathbf{V}\cdot\mathbf{v} = 0$ on Γ. See Figure 1 for an illustration.

In order to close the model, a relation between η and u must be specified, which plays the role of a constitutive relation that takes into account adhesion properties of the aptamer. First of all, the adhered protein molecules are not being released any more. Moreover, there exist two thresholds u_0 and u_1 such that the aptamer cannot bind protein molecules both, if $u|_\Gamma \leqslant u_0$ (insufficient concentration for the activation) and, if $u|_\Gamma \geqslant u_1$ (exhaustion of free aptamer molecules). The constitutive relation looks as follows:

$$\eta(x,t) = \mathscr{A}(u(x,\cdot))(t), \quad x \in \Gamma, \ t \in (0,T) \tag{6}$$

where $\mathscr{A}$ is a hysteresis operator defined on $L^\infty(0,T)$ by the relation

$$\mathscr{A}(\xi)(t) = \operatorname{ess\,sup}\{H(\xi(\tau)) : \tau \leqslant t\}, \quad \xi \in L^\infty(0,T) \tag{7}$$

where the function H is defined as in Figure 2(a). The action of the operator $\mathscr{A}$ is schematically shown in Figure 2(b).

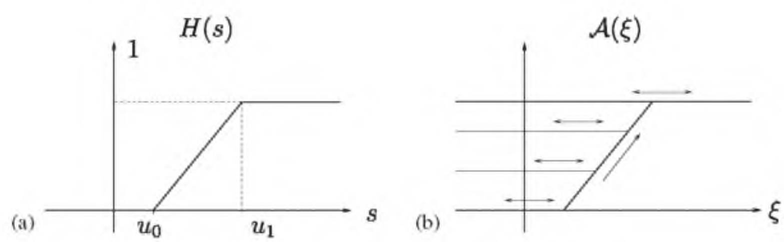

Figure 2. Schematic representation of the operator $\mathscr{A}$.

Remark 1.1
A simplified notation $\eta = \mathscr{A}(u)$ will be used instead of (6), i.e. the arguments will be omitted whenever this does not lead to a confusion. Moreover, note that the surface concentration of the protein η assumes values from the interval $[0,1]$, whereas the rescaled protein volume fraction u is of the order 1 but can exceed 1.

In order to reduce the diffusion coefficient to 1, rescale the time variable by multiplying it by α (see formula (1)). In the new variables (the old notation is kept for the rescaled time and fluid velocity), our problem is rewritten as follows:

$$\Omega \times [0,T]: \quad u_t = \Delta u - \operatorname{div}(u\mathbf{V}) \tag{8}$$

$$\partial\Omega \setminus \Gamma \times [0,T]: \quad \frac{\partial u}{\partial \mathbf{v}} = 0 \tag{9}$$

$$\Gamma \times [0,T]: \quad \eta_t = -\frac{\partial u}{\partial \mathbf{v}}, \quad \eta = \mathscr{A}(u) \tag{10}$$

$$t = 0: \quad u = u^0, \quad \eta = \eta^0 \tag{11}$$

where $\mathscr{A}$ is defined by (7), see also (6) and Remark 1.1. Assume that the velocity $\mathbf{V}$ is sufficiently smooth, bounded, i.e. $|\mathbf{V}(x,t)| \leqslant C$, and satisfies the conditions: $\operatorname{div}\mathbf{V} = 0$ and $\mathbf{V}\cdot\mathbf{v}|_{\partial\Omega\setminus(\Gamma^{\text{in}}\cup\Gamma^{\text{out}})} = 0$. Suppose for simplicity that $\mathbf{V}$ is time independent on Γ^{in} and Γ^{out}.
Problems (8)–(11) is called *Problem A*.

1.2. Main result

Definition 1.2
A pair of functions

$$u \in H^1(\Omega_T), \quad \eta \in L^\infty(\Gamma_T)$$

with $u|_{t=0} = u^0$ is called a generalized solution to *Problem A*, if

$$\eta(\mathbf{x},t) = \mathscr{A}(u(\mathbf{x},\cdot))(t) \quad \text{for almost all } (\mathbf{x},t) \in \Gamma_T \tag{12}$$

and the following integral identity

$$\int_0^T \int_\Omega [u_t\psi + \nabla u \nabla \psi - u\mathbf{V}\nabla\psi]\,\mathrm{d}\mathbf{x}\,\mathrm{d}t + \int_0^T \int_{\Gamma^{\text{in}}} g\psi(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s\,\mathrm{d}t + \int_0^T \int_{\Gamma^{\text{out}}} u\psi(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s\,\mathrm{d}t$$
$$-\int_0^T \int_\Gamma \eta\psi_t\,\mathrm{d}s\,\mathrm{d}t - \int_\Gamma \eta^0\psi^0\,\mathrm{d}s = 0 \tag{13}$$

holds for every smooth function ψ such that $\psi|_{t=T} = 0$.

Here $\Omega_T = \Omega \times [0,T]$, $\Gamma_T = \Gamma \times [0,T]$, $\psi^0 = \psi|_{t=0}$, $\mathrm{d}s$ denotes the two-dimensional Lebesgue measure, η^0 is a weak initial condition for η.
The following theorem is the main result of this paper.

Theorem 1.3
Let $u^0 \in H^1(\Omega)\cap L^\infty(\Omega)$, $u^0 \geqslant 0$, $g \in L^\infty(\Gamma^{\text{in}})$, and η^0 is a measurable function such that $\eta^0(\mathbf{x}) = H(u^0(\mathbf{x}))$ for $\mathbf{x}\in\Gamma$. Then there exists a unique generalized solution to *Problem A* such that

$$u_t, \Delta u \in L^2(\Omega_T), \quad u_{x_\sigma} \in L^\infty(0,T; L^2(\Omega)), \quad \sigma = 1,2,3$$

$$0 \leqslant u \leqslant \max\{\|u^0\|_{L^\infty(\Omega)}, \|g\|_{L^\infty(\Gamma^{\text{in}})}\}$$

$$\eta_t \in L^2(\Gamma_T), \quad \eta \in H^{1/2}(\Gamma_T)$$

Remark 1.4
The condition $\eta^0 = H(u^0)$ has a physical sense and, besides that, simplifies some mathematical calculations. Nevertheless, it is not important and can be relaxed.

Remark 1.5
The integral $\int_{\Gamma^{\text{in}}} g(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s$ in (13) represents the mass flux of the protein at the inlet scaled by $\delta\phi_{\max}$ according to (2). It is observed in [2, 7.6] that the equality $u = g$ holds on Γ^{in} for any $t > 0$, if it holds at $t = 0$. A physical explanation of this effect is that the reasonable range of the diffusion coefficient α is about 10^{-5}–10^{-7}, whereas the magnitude of the velocity $\mathbf{V}$ on the inlet is of the order of 10^{-2}–1, and $\mathbf{V}$ is nearly parallel to $\mathbf{v}$, except for a very small region near the relative boundary of Γ^{in}. Therefore, the diffusion mass flux $-\alpha\nabla(\rho_p\phi)\cdot\mathbf{v}$ is strongly dominated by the transport term $(\rho_p\phi)\mathbf{V}\cdot\mathbf{v}$ near the inlet unless the gradient assumes nonphysically large values. Thus, if g is the trace of u^0 on Γ^{in} at $t = 0$, then the trace of u stays very close to g for $t > 0$. Numerous numerical experiments confirm this effect. Therefore, using the assumption that $\operatorname{div}\mathbf{V} = 0$, the integral identity (13) can be replaced by the following one:

$$\int_0^T \int_\Omega (u_t\psi + \nabla u\cdot\nabla\psi + \mathbf{V}\cdot\nabla u\psi)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t - \int_0^T \int_\Gamma \eta\psi_t\,\mathrm{d}s\,\mathrm{d}t + \int_\Gamma \eta^0\psi^0\,\mathrm{d}s = 0 \tag{14}$$

1.3. *Bibliographical remarks*

Problems with hysteresis have been considered in numerous publications. We refer to the books [3–6] for surveys in this area. The common feature of investigations cited there is the regularizing term $\varepsilon\partial u/\partial t$ added to the boundary condition (10) to improve the regularity of $u|_\Gamma$ with respect to t. Thus, the boundary condition on Γ would be transformed to

$$\varepsilon\frac{\partial u}{\partial t} + \eta_t = -\frac{\partial u}{\partial \mathbf{v}}, \quad \eta = \mathscr{A}(u)$$

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

2. PROOF OF THE MAIN RESULT

The proof of Theorem 1.3 is rather complicated technically and demands many estimations, auxiliary results, and accounting for fine properties of solutions to parabolic partial differential equations (PDEs) stated, e.g. in [7].

2.1. *Construction of approximate solutions*

Use the implicit time discretization scheme to approximate Problem (8)–(11). Fix arbitrary $N\in\mathbb{N}$ and set $\tau=T/N$. Define functions u^n, $n\in\{1,2,\dots,N\}$ as solutions of the following problem:

$$u^n-u^{n-1}=\tau\Delta u^n-\tau\mathbf{V}\cdot\nabla u^n,\quad \mathbf{x}\in\Omega \tag{15}$$

$$\eta^n-\eta^{n-1}=-\tau\frac{\partial u^n}{\partial\mathbf{v}},\quad \mathbf{x}\in\Gamma \tag{16}$$

$$\frac{\partial u^n}{\partial\mathbf{v}}=0,\quad \mathbf{x}\in\partial\Omega\setminus\Gamma \tag{17}$$

where

$$\eta^n(\mathbf{x})=\max_{k\in\{0,1,\dots,n\}}H(u^k(\mathbf{x})),\quad \mathbf{x}\in\Gamma \tag{18}$$

Note that

$$\eta^n(\mathbf{x})=\eta^{n-1}(\mathbf{x})+(H(u^n(\mathbf{x}))-\eta^{n-1}(\mathbf{x}))^+,\quad \mathbf{x}\in\Gamma \tag{19}$$

where as usual, $f^+:=\max(0,f)$.

Lemma 2.1
If τ is sufficiently small, the problem (15)–(17) are uniquely solvable with respect to u^n.

Proof
Define operator $A(u,v):H^1(\Omega)\times H^1(\Omega)\to(H^1(\Omega))'$ as follows:

$$\langle A(u,v),\phi\rangle=\int_\Omega v\phi\,\mathbf{dx}+\tau\int_\Omega\nabla v\nabla\phi\,\mathbf{dx}+\int_\Gamma(H(v)-\eta^{n-1})^+\phi\,\mathrm{d}s+\tau\int_\Omega\mathbf{V}\cdot\nabla u\phi\,\mathbf{dx}$$

where $\phi\in H^1(\Omega)$ is an arbitrary function, and $\langle\cdot,\cdot\rangle$ denotes the duality product between $(H^1(\Omega))'$ and $H^1(\Omega)$. It is easy to prove that the operator $A(u,v)$ satisfies all conditions of Definition 2.2 of [8], so that the operator $A(u)=A(u,u)$ is a variational one in the sense of this definition. Let a functional $f\in(H^1(\Omega))'$ is defined by

$$\langle f,\phi\rangle=\int_\Omega u^{n-1}\phi\,\mathbf{dx},\quad \phi\in H^1(\Omega)$$

According to Corollary 2.1 of [8], the equation $A(u)=f$ has at least one solution. Prove now the uniqueness of such a solution. Assume, there are two solutions u_1 and u_2. Denote $\bar{u}:=u_1-u_2$. Then

$$\langle A(u_1)-A(u_2),u_1-u_2\rangle=\int_\Omega(\bar{u})^2\,\mathbf{dx}+\tau\int_\Omega(\nabla\bar{u})^2\,\mathbf{dx}\int_\Gamma[(H(u_1)-\eta^{n-1})^+$$
$$-(H(u_2)-\eta^{n-1})^+][u_1-u_2]\,\mathrm{d}s+\tau\int_\Omega\mathbf{V}\cdot\nabla\bar{u}\bar{u}\,\mathbf{dx}=0$$

Taking into account that the integral over Γ is nonnegative, yields for any $\varepsilon>0$:

$$\int_\Omega (\bar{u})^2\,\mathrm{d}\mathbf{x}+\tau\int_\Omega (\nabla\bar{u})^2\,\mathrm{d}\mathbf{x}\leqslant\tau\varepsilon C^2\int_\Omega(\nabla\bar{u})^2\,\mathrm{d}\mathbf{x}+\frac{\tau}{\varepsilon}\int_\Omega(\bar{u})^2\,\mathrm{d}\mathbf{x}$$

Choosing $\varepsilon<1/C^2$ and assuming that $\tau<\varepsilon$ implies that $\bar{u}=0$. □

Lemma 2.2
Let $\mathbf{V}$ be a smooth vector function satisfying the following conditions: $|\mathbf{V}(x,t)|\leqslant C$, $\operatorname{div}\mathbf{V}=0$, and

$$\mathbf{V}\cdot\mathbf{v}\leqslant 0 \quad \text{on } \Gamma^{\mathrm{in}}$$

$$\mathbf{V}\cdot\mathbf{v}\geqslant 0 \quad \text{on } \Gamma^{\mathrm{out}}$$

$$\mathbf{V}\cdot\mathbf{v}=0 \quad \text{else}$$

Then, for all functions $\xi,\psi\in H^1(\Omega)$, the following relations hold:

$$\int_\Omega \mathbf{V}\cdot\nabla\xi\psi\,\mathrm{d}\mathbf{x}=\int_{\Gamma^{\mathrm{in}}\cup\Gamma^{\mathrm{out}}}\xi\psi(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s-\int_\Omega\mathbf{V}\cdot\nabla\psi\xi\,\mathrm{d}\mathbf{x}$$

$$\int_\Omega \mathbf{V}\cdot\nabla\xi\xi\,\mathrm{d}\mathbf{x}=\frac{1}{2}\int_{\Gamma^{\mathrm{in}}\cup\Gamma^{\mathrm{out}}}\xi^2(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s\geqslant\frac{1}{2}\int_{\Gamma^{\mathrm{in}}}\xi^2(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s$$

$$-\int_\Omega \mathbf{V}\cdot\nabla\xi\xi\,\mathrm{d}\mathbf{x}\leqslant\frac{1}{2}\int_{\Gamma^{\mathrm{in}}}\xi^2|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s$$

The proof is obvious because $\mathbf{V}\cdot\mathbf{v}\geqslant 0$ on Γ^{out} and $\mathbf{V}\cdot\mathbf{v}\leqslant 0$ on Γ^{in}.

Lemma 2.3
Let $f:\mathbb{R}\to\mathbb{R}$ be a C^1 function such that f' does not decrease. Then

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

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

Proof
Really, if $\alpha>\beta$, then $f(\alpha)-f(\beta)=f'(\xi_0)(\alpha-\beta)\leqslant f'(\alpha)(\alpha-\beta)$, where $\xi_0\in[\beta,\alpha]$. If $\alpha<\beta$, then $f(\beta)-f(\alpha)=f'(\xi_0)(\beta-\alpha)\geqslant f'(\alpha)(\beta-\alpha)$, where $\xi_0\in[\alpha,\beta]$. □

Lemma 2.4
Let u^0,η^0, and g be nonnegative and bounded. Then, for all $n=1,2,\ldots,N$ and for almost all $\mathbf{x}\in\Omega$, the following estimate holds:

$$0\leqslant u^n(\mathbf{x})\leqslant\max\{\|u^0\|_{L^\infty(\Omega)},\|g\|_{L^\infty(\Gamma^{\mathrm{in}})}\}$$

Proof

Denote $b=\max\{\|u^0\|_{L^\infty(\Omega)}, \|g\|_{L^\infty(\Gamma^{\text{in}})}\}$ and introduce the function

$$f(\xi)=\begin{cases}\xi^2, & \xi\leqslant 0\\ 0, & 0\leqslant\xi\leqslant b\\ (\xi-b)^2, & \xi\geqslant b\end{cases}$$

It is not difficult to see that this function satisfies the conditions of Lemma 2.3. Multiply (15) by $f'(u^n)$ and integrate over Ω to obtain that

$$\int_\Omega\left(f'(u^n)\frac{u^n-u^{n-1}}{\tau}+f''(u^n)|\nabla u^n|^2+\mathbf{V}\cdot\nabla u^n f'(u^n)\right)\mathrm{d}\mathbf{x}$$
$$=\int_\Gamma\frac{\partial u^n}{\partial\mathbf{v}}f'(u^n)\,\mathrm{d}s=-\int_\Gamma\frac{\eta^n-\eta^{n-1}}{\tau}f'(u^n)\,\mathrm{d}s\leqslant 0 \qquad (20)$$

because the function $(\eta^n-\eta^{n-1})f'(u^n)$ is nonnegative on Γ.

Really, if $u^n(\mathbf{x})\geqslant 0$, then $f'(u^n(\mathbf{x}))\geqslant 0$. Then the obvious inequality $\eta^n\geqslant\eta^{n-1}$ implies that $(\eta^n(\mathbf{x})-\eta^{n-1}(\mathbf{x}))f'(u^n(\mathbf{x}))\geqslant 0$. If $u^n(\mathbf{x})\leqslant 0$, then $\eta^n(\mathbf{x})=\eta^{n-1}(\mathbf{x})$ (see (19) and take into account that all η^i are nonnegative because u^0 is nonnegative). Explicit computations yield $\nabla u^n f'(u^n)=1/2\nabla f'(u^n)f'(u^n)$. Therefore, $\int_\Omega\mathbf{V}\cdot\nabla u^n f'(u^n)\,\mathrm{d}\mathbf{x}\geqslant 1/4\int_{\Gamma^{\text{in}}}f'(u^n)^2(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s$ due to Lemma 2.2. Using (20), Lemma 2.3, and the convexity of the function f yields:

$$\int_\Omega f(u^n)\,\mathrm{d}\mathbf{x}\leqslant\int_\Omega f(u^{n-1})\,\mathrm{d}\mathbf{x}-\frac{\tau}{4}\int_{\Gamma^{\text{in}}}|f'(u^n)|^2(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s$$

The choice of b and the relation $u^n|_{\Gamma^{\text{in}}}=g$ imply that $f'(u^n)|_{\Gamma^{\text{in}}}=0$. Therefore, taking again into account the choice of b implies that $\int_\Omega f(u^n)\,\mathrm{d}\mathbf{x}=0$, which proves the lemma. □

Define $\|g\|^2_{L^2(\Gamma^{\text{in}};|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s)}:=\int_{\Gamma^{\text{in}}}g^2|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s\leqslant C\|g\|^2_{L^\infty(\Gamma^{\text{in}})}\mathrm{meas}(\Gamma^{\text{in}})$.

Lemma 2.5

The following estimate holds:

$$\frac{1}{2}\int_\Omega|u^n|^2\,\mathrm{d}\mathbf{x}+\tau\sum_{k=1}^n\int_\Omega|\nabla u^k|^2\,\mathrm{d}\mathbf{x}\leqslant\frac{1}{2}\int_\Omega|u^0|^2\,\mathrm{d}\mathbf{x}+\frac{T}{2}\|g\|^2_{L^2(\Gamma^{\text{in}};|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s)}$$

Proof

Multiplying (15) by u^n yields

$$\int_\Omega((u^n-u^{n-1})u^n+\tau|\nabla u^n|^2+\tau\mathbf{V}\nabla u^n u^n)\,\mathrm{d}\mathbf{x}=-\int_\Gamma(H(u^n)-\eta^{n-1})^+u^n\,\mathrm{d}s$$

Obviously

$$\int_\Omega(u^n-u^{n-1})u^n\,\mathrm{d}\mathbf{x}=\frac{1}{2}\int_\Omega|u^n|^2\,\mathrm{d}\mathbf{x}-\frac{1}{2}\int_\Omega|u^{n-1}|^2\,\mathrm{d}\mathbf{x}+\frac{1}{2}\int_\Omega|u^n-u^{n-1}|^2\,\mathrm{d}\mathbf{x}$$

Taking into account that $-2\int_\Omega \mathbf{V}\cdot\nabla u^n u^n \leqslant \int_{\Gamma^{\mathrm{in}}} g^2|\mathbf{V}\cdot\boldsymbol{\nu}|\,\mathrm{d}s$ (Lemma 2.2) and $(H(u^n)-\eta^{n-1})^+u^n \geqslant 0$ (Lemma 2.4) yields

$$\frac{1}{2}\int_\Omega |u^n|^2\,\mathrm{d}\mathbf{x}+\tau\sum_{k=1}^{n}\int_\Omega |\nabla u^k|^2\,\mathrm{d}\mathbf{x}\leqslant \frac{1}{2}\int_\Omega |u^0|^2\,\mathrm{d}\mathbf{x}+\frac{T}{2}\|g\|^2_{L^2(\Gamma^{\mathrm{in}};|\mathbf{V}\cdot\boldsymbol{\nu}|\,\mathrm{d}s)} \qquad \square$$

Definition 2.6
Define

$$B:=\int_\Omega |\nabla u^0|^2\,\mathrm{d}\mathbf{x}+\frac{C^2}{2}\int_\Omega |u^0|^2\,\mathrm{d}\mathbf{x}+\frac{C^2T}{2}\|g\|^2_{L^2(\Gamma^{\mathrm{in}};|\mathbf{V}\cdot\boldsymbol{\nu}|\,\mathrm{d}s)}$$

with $C:=\|\mathbf{V}\|_{L^\infty(\Omega_T)}$.

Lemma 2.7
The following estimate holds:

$$\frac{1}{2}\sum_{k=1}^{n}\tau\int_\Omega\left|\frac{u^k-u^{k-1}}{\tau}\right|^2\mathrm{d}\mathbf{x}+\frac{1}{2}\int_\Omega|\nabla u^n|^2\,\mathrm{d}\mathbf{x}\leqslant\frac{B}{2} \tag{21}$$

Proof
Multiplying (15) by u^n-u^{n-1} yields:

$$\tau\int_\Omega\left|\frac{u^n-u^{n-1}}{\tau}\right|^2\mathrm{d}\mathbf{x}+\int_\Omega \nabla u^n(\nabla u^n-\nabla u^{n-1})\,\mathrm{d}\mathbf{x}=-\int_\Gamma (H(u^n)-\eta^{n-1})^+(u^n-u^{n-1})\,\mathrm{d}s$$
$$-\tau\int_\Omega \mathbf{V}\cdot\nabla u^n\left(\frac{u^n-u^{n-1}}{\tau}\right)\mathrm{d}\mathbf{x} \tag{22}$$

If $u^n(x)\leqslant u^{n-1}(x)$, then $H(u^n(x))\leqslant\eta^{n-1}(x)$ and, therefore, $(H(u^n(x))-\eta^{n-1}(x))^+=0$. Thus, $(H(u^n)-\eta^{n-1})^+(u^n-u^{n-1})\geqslant 0$ for all $x\in\Gamma$. Taking into account the identity

$$\int_\Omega \nabla u^n(\nabla u^n-\nabla u^{n-1})\,\mathrm{d}\mathbf{x}=\frac{1}{2}\int_\Omega|\nabla u^n|^2\,\mathrm{d}\mathbf{x}-\frac{1}{2}\int_\Omega|\nabla u^{n-1}|^2\,\mathrm{d}\mathbf{x}+\frac{1}{2}\int_\Omega|\nabla u^n-\nabla u^{n-1}|^2\,\mathrm{d}\mathbf{x}$$

the estimate

$$\left|\int_\Omega \mathbf{V}\cdot\nabla u^n\left(\frac{u^n-u^{n-1}}{\tau}\right)\mathrm{d}\mathbf{x}\right|\leqslant\frac{C^2}{2\varepsilon}\int_\Omega|\nabla u^n|^2\,\mathrm{d}\mathbf{x}+\frac{\varepsilon}{2}\int_\Omega\left|\frac{u^n-u^{n-1}}{\tau}\right|^2\mathrm{d}\mathbf{x}$$

with $\varepsilon=1$, and Lemma 2.5, we obtain from (22):

$$\frac{1}{2}\sum_{k=1}^{n}\tau\int_\Omega\left|\frac{u^k-u^{k-1}}{\tau}\right|^2\mathrm{d}\mathbf{x}+\frac{1}{2}\int_\Omega|\nabla u^n|^2\,\mathrm{d}\mathbf{x}\leqslant\frac{B}{2} \qquad \square$$

Further, Equation (15), Lemmas 2.5 and 2.7 imply:

$$\sum_{k=1}^{n}\tau\int_\Omega|\Delta u^k|^2\,\mathrm{d}\mathbf{x}\leqslant\sum_{k=1}^{n}\tau\int_\Omega\left[2\left|\frac{u^k-u^{k-1}}{\tau}\right|^2+2C^2|\nabla u^k|^2\right]\mathrm{d}\mathbf{x}$$
$$\leqslant 2\int_\Omega|\nabla u^0|^2\,\mathrm{d}\mathbf{x}+2C^2\int_\Omega|u^0|^2\,\mathrm{d}\mathbf{x}+2C^2T\|g\|^2_{L^2(\Gamma^{\mathrm{in}};|\mathbf{V}\cdot\boldsymbol{\nu}|\,\mathrm{d}s)} \tag{23}$$

Obtain some other estimates. Define

$$\zeta^n(\mathbf{x}) := \max_{k\in\{0,1,\ldots,n\}} H(u^k(\mathbf{x})), \quad \mathbf{x}\in\Omega \tag{24}$$

Note that another equivalent definition of this function is the following:

$$\zeta^n(\mathbf{x}) := \zeta^{n-1}(\mathbf{x}) + (H(u^n(\mathbf{x})) - \zeta^{n-1}(\mathbf{x}))^+, \quad \mathbf{x}\in\Omega \tag{25}$$

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

$$\eta^n = \gamma_0 \zeta^n \tag{26}$$

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

Lemma 2.8
For all $n=1,2,\ldots,N$, the following estimates hold:

$$\int_\Omega |\nabla\zeta^n|^2\,\mathrm{d}\mathbf{x} \leqslant c_0^2 B \tag{27}$$

$$\sum_{k=1}^{n} \tau \int_\Omega \left(\frac{\zeta^k - \zeta^{k-1}}{\tau}\right)^2 \mathrm{d}\mathbf{x} \leqslant c_0^2 B \tag{28}$$

$$\sum_{k=1}^{n} \tau \int_\Gamma \left(\frac{\eta^k - \eta^{k-1}}{\tau}\right)^2 \mathrm{d}s \leqslant \frac{c_0}{2} B \tag{29}$$

where $c_0 = \max_{s\in\mathbb{R}}(\mathrm{d}H(s)/\mathrm{d}s)$.

Proof
Denote

$$\xi^n(\mathbf{x}) = \max_{k\in\{0,1,\ldots,n\}} u^k(\mathbf{x}), \quad \mathbf{x}\in\Omega$$

It is not difficult to see that $\zeta^n = H(\xi^n)$. Let G^n be the subset of Ω where $u^n \geqslant \xi^{n-1}$.
Multiplying (15) by $\xi^n - \xi^{n-1}$ yields:

$$\int_\Omega ((u^n - u^{n-1})(\xi^n - \xi^{n-1}) + \tau\nabla u^n\cdot\nabla(\xi^n - \xi^{n-1}) + \tau\mathbf{V}\cdot\nabla u^n(\xi^n - \xi^{n-1}))\,\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma (\eta^n - \eta^{n-1})(\xi^n - \xi^{n-1})\,\mathrm{d}s = 0$$

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

$$\int_\Omega (\xi^n - \xi^{n-1})^2\,\mathrm{d}\mathbf{x} + \int_\Gamma (\eta^n - \eta^{n-1})(\xi^n - \xi^{n-1})\,\mathrm{d}s + \tau\int_\Omega \nabla u^n\cdot\nabla(\xi^n - \xi^{n-1})\,\mathrm{d}\mathbf{x}$$
$$\leqslant \frac{C^2\tau^2}{2}\int_\Omega |\nabla u^n|^2 + \frac{1}{2}\int_\Omega (\xi^n - \xi^{n-1})^2\,\mathrm{d}\mathbf{x} \tag{30}$$

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,

$$\begin{aligned}\int_\Omega \nabla u^n\cdot\nabla(\xi^n-\xi^{n-1})\,\mathrm{d}\mathbf{x} &= \int_{G^n}\nabla u^n\cdot\nabla(\xi^n-\xi^{n-1})\,\mathrm{d}\mathbf{x}\\ &= \int_{G^n}\nabla\xi^n\cdot\nabla(\xi^n-\xi^{n-1})\,\mathrm{d}\mathbf{x} = \int_\Omega\nabla\xi^n\cdot\nabla(\xi^n-\xi^{n-1})\,\mathrm{d}\mathbf{x}\\ &= \frac{1}{2}\int_\Omega|\nabla\xi^n|^2\,\mathrm{d}\mathbf{x}-\frac{1}{2}\int_\Omega|\nabla\xi^{n-1}|^2\,\mathrm{d}\mathbf{x}+\frac{1}{2}\int_\Omega|\nabla\xi^n-\nabla\xi^{n-1}|^2\,\mathrm{d}\mathbf{x}\end{aligned}$$

Estimating (30) together with the last relation and Lemma 2.5 yields:

$$\begin{aligned}&\frac{1}{\tau}\sum_{k=1}^n\int_\Omega(\xi^k-\xi^{k-1})^2\,\mathrm{d}\mathbf{x}+\frac{2}{\tau}\sum_{k=1}^n\int_\Gamma(\eta^k-\eta^{k-1})(\xi^k-\xi^{k-1})\,\mathrm{d}s+\int_\Omega|\nabla\xi^n|^2\,\mathrm{d}\mathbf{x}\\ &\quad\leqslant\int_\Omega|\nabla\xi^0|^2\,\mathrm{d}\mathbf{x}+\frac{C^2}{2}\int_\Omega|u^0|^2\,\mathrm{d}\mathbf{x}+\frac{C^2T}{2}\|g\|^2_{L^2(\Gamma^{\mathrm{in}};|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s)}\end{aligned}$$

Note that $\zeta^k-\zeta^{k-1}=H(\xi^k)-H(\xi^{k-1})\leqslant c_0(\xi^k-\xi^{k-1})$, where $c_0=\max_{s\in\mathbb{R}}(\mathrm{d}H(s)/\mathrm{d}s)>0$. Therefore, multiplying the last estimate by c_0^2 yields:

$$\frac{1}{\tau}\sum_{k=1}^n\int_\Omega(\zeta^k-\zeta^{k-1})^2\,\mathrm{d}\mathbf{x}+\frac{2c_0}{\tau}\sum_{k=1}^n\int_\Gamma(\eta^k-\eta^{k-1})^2\,\mathrm{d}s+c_0^2\int_\Omega|\nabla\xi^n|^2\,\mathrm{d}\mathbf{x}\leqslant c_0^2B$$

The assertion of the lemma follows immediately from this inequality together with $\nabla\zeta^n=H'(\xi^n)\nabla\xi^n$. □

2.2. *Passage to the limit*

For every $N\in\mathbb{N}$, define two kinds of time interpolations of $\{u^n\}$, $\{\eta^n\}$, and $\{\zeta^n\}$. Let u_N, η_N, and ζ_N be piecewise linear interpolations, whereas $\overline{u}_N$, $\overline{\eta}_N$, and $\overline{\zeta}_N$ are piecewise constant ones. That is,

$$u_N(\mathbf{x},t)=u^n(\mathbf{x})\left(1-n+\frac{t}{\tau}\right)+u^{n-1}(\mathbf{x})\left(n-\frac{t}{\tau}\right)\quad\text{if } t\in[(n-1)\tau,n\tau],\quad n=1,\ldots,N$$

$$\overline{u}_N(\mathbf{x},t)=u^n(\mathbf{x})\quad\text{if } t\in((n-1)\tau,n\tau],\quad n=1,\ldots,N$$

The functions η_N, ζ_N, $\overline{\eta}_N$, and $\overline{\zeta}_N$ are defined in the same way.

Lemma 2.9

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

as $N\to\infty$.

Proof
Owing to estimate (21), the following is true

$$\int_0^T \|u_N(t)-\overline{u}_N(t)\|^2_{L^2(\Omega)}\,\mathrm{d}t=\sum_{n=1}^N \|u^n-u^{n-1}\|^2_{L^2(\Omega)}\int_{(n-1)\tau}^{n\tau}\left(\frac{t}{\tau}-n\right)^2\,\mathrm{d}t$$

$$=\frac{\tau}{3}\sum_{n=1}^N \|u^n-u^{n-1}\|^2_{L^2(\Omega)}\leqslant\frac{\tau^2 B}{3}$$

which proves the first assertion of the lemma because $\tau=T/N$. The other two claims can be proved using the same arguments and estimates (28) and (29). □

Estimates (21), (23), (27), (28), and (29) imply:

$$\begin{gathered}\left\|\frac{\partial u_N}{\partial t}\right\|^2_{L^2(\Omega_T)},\ \|\nabla u_N\|^2_{L^\infty(0,T;L^2(\Omega))},\ \|\nabla \overline{u}_N\|^2_{L^\infty(0,T;L^2(\Omega))}\leqslant B\\ \left\|\frac{\partial \eta_N}{\partial t}\right\|^2_{L^2(\Gamma_T)}\leqslant\frac{c_0 B}{2}\\ \left\|\frac{\partial \zeta_N}{\partial t}\right\|^2_{L^2(\Omega_T)},\ \|\nabla \zeta_N\|^2_{L^\infty(0,T;L^2(\Omega))},\ \|\nabla \overline{\zeta}_N\|^2_{L^\infty(0,T;L^2(\Omega))}\leqslant c_0^2 B\\ \|\Delta u_N\|^2_{L^2(\Omega_T)}\leqslant 2\|\nabla u^0\|^2_{L^2(\Omega)}+2C^2\|u^0\|_{L^2(\Omega)}+2C^2T\|g\|^2_{L^2(\Gamma^{\mathrm{in}};\,|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s)}\end{gathered}\tag{31}$$

Equations (15)–(18), under accounting for estimates (31), yield:

$$\frac{\partial u_N}{\partial t}=\Delta\overline{u}_N-\mathbf{V}\cdot\nabla\overline{u}_N\quad \text{in } L^2(\Omega_T)\tag{32}$$

$$\frac{\partial \eta_N}{\partial t}=-\frac{\partial \overline{u}_N}{\partial \mathbf{v}}\quad \text{in } L^2(0,T;H^{-1/2}(\Gamma))\tag{33}$$

$$\frac{\partial \overline{u}_N}{\partial \mathbf{v}}=0\quad \text{in } L^2(0,T;H^{-1/2}(\partial\Omega\setminus\Gamma))\tag{34}$$

$$\overline{\eta}_N(\mathbf{x},t)=\mathscr{A}(\overline{u}_N(\mathbf{x},\cdot))(t)\quad \text{for a.a. } (\mathbf{x},t)\in\Gamma_T\tag{35}$$

$$\overline{\zeta}_N(\mathbf{x},t)=\mathscr{A}(\overline{u}_N(\mathbf{x},\cdot))(t)\quad \text{for a.a. } (\mathbf{x},t)\in\Omega_T\tag{36}$$

Additionally, relation (26) implies:

$$\overline{\eta}_N=\gamma_0\overline{\zeta}_N\quad \text{in } L^\infty(0,T;H^{1/2}(\Gamma))\tag{37}$$

Owing to estimates (31) and Lemma 2.9, there exists a sequence $N_m\to\infty$ and functions u, η, and ζ such that

$$u_{N_m}\to u\quad *\text{-weakly in } H^1(0,T;L^2(\Omega))\cap L^\infty(0,T;H^1(\Omega))$$

$$\overline{u}_{N_m}\to u\quad *\text{-weakly in } L^\infty(0,T;H^1(\Omega))$$

$$\zeta_{N_m} \to \zeta \quad *\text{-weakly in } H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega))$$

$$\overline{\zeta}_{N_m} \to \zeta \quad *\text{-weakly in } L^\infty(0,T;H^1(\Omega))$$

$$\eta_{N_m} \to \eta \quad \text{weakly in } H^1(0,T;L^2(\Gamma))$$

$$\overline{\eta}_{N_m} \to \eta \quad *\text{-weakly in } L^\infty(0,T;H^{1/2}(\Gamma))$$

As a corollary, the limiting functions possess the properties:

$$u \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad \Delta u \in L^2(\Omega_T)$$

$$\zeta \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega))$$

$$\eta \in H^1(0,T;L^2(\Gamma)) \cap L^\infty(0,T;H^{1/2}(\Gamma))$$

Moreover, the functions u, η, and ζ are bounded due to Lemma 2.4, and the estimate holds:

$$0 \leqslant u(\mathbf{x},t) \leqslant \max\{\|u^0\|_{L^\infty(\Omega)}, \|g\|_{L^\infty(\Gamma^{\text{in}})}\}$$

The passage to the limit with respect to the subsequences in (32)–(34), and (37) yields:

$$\frac{\partial u}{\partial t} = \Delta u - \mathbf{V} \cdot \nabla u \quad \text{in } L^2(\Omega_T) \tag{38}$$

$$\frac{\partial \eta}{\partial t} = -\frac{\partial u}{\partial \mathbf{v}} \quad \text{in } L^2(0,T;H^{-1/2}(\Gamma)) \tag{39}$$

$$\frac{\partial u}{\partial \mathbf{v}} = 0 \quad \text{in } L^2(0,T;H^{-1/2}(\partial\Omega \backslash \Gamma)) \tag{40}$$

$$\eta = \gamma_0 \zeta \quad \text{in } L^\infty(0,T;H^{1/2}(\Gamma)) \tag{41}$$

In order to prove the existence of a solution to *Problem A*, it is necessary to establish (12). First, prove that

$$\zeta(\mathbf{x},t) = \mathscr{A}(u(\mathbf{x},\cdot))(t) \quad \text{for almost all } (\mathbf{x},t) \in \Omega_T \tag{42}$$

This can be done almost in the same way as in [4, IX.1]. Note that, for every $s \in (0, \frac{1}{2})$ the following embeddings are true:

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

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

$$\mathscr{A}(\overline{u}_{N_m}(\mathbf{x},\cdot))(t) = \operatorname*{ess\,sup}_{s\in[0,t]} H(\overline{u}_{N_m}(\mathbf{x},s)) = \operatorname*{ess\,sup}_{s\in[0,n\tau]} H(\overline{u}_{N_m}(\mathbf{x},s))$$

$$= \max_{s\in[0,n\tau]} H(u_{N_m}(\mathbf{x},s)) = \max_{s\in[0,t]} H(u_{N_m}(\mathbf{x},s)) + R(\tau, u_{N_m}, t)$$

where $|R(\tau, u_{N_m}, t)| \leqslant C\tau^\alpha$ with a constant C, which is independent on N_m and t. The passage to the limit in (36) then yields (42).

In view of (41) and (42), it only remains to prove that

$$\gamma_0 \mathscr{A}(u)(t) = \mathscr{A}(\gamma_0 u)(t) \quad \text{for almost all } t \in [0,T] \tag{43}$$

where u is the limit of $\{u_{N_m}\}$. In order to do that, it is necessary to establish some additional regularity properties of the function u.

Lemma 2.10
For every $\delta > 0$, there exists $\alpha \in (0,1)$ such that $u \in C^{\alpha,\alpha/2}(\overline{Q})$, where Q is an arbitrary domain in Ω_T such that $\overline{Q} \subset \overline{\Omega}_T$ and $\operatorname{dist}(Q, \{(\mathbf{x},t) \in \mathbb{R}^{3+1} | t=0\}) > \delta$.

Proof
The assertion of the lemma follows (not quite immediately) from techniques of [7, III.10]. To apply them, the a.e. boundedness of solutions should be proved. Let us take an arbitrary number $k > \|g\|_{L^\infty(\Gamma^{\text{in}})}$ and multiply (38) by $(u-k)^+$. After integration over Ω and taking into account that $-2\int_\Omega \mathbf{V} \cdot \nabla u (u-k)^+ \leqslant \int_{\Gamma^{\text{in}}} ((g-k)^+)^2 |\mathbf{V} \cdot \mathbf{v}| \, \mathrm{d}s$ because $\nabla u (u-k)^+ = \nabla (u-k)^+ (u-k)^+$ a.e. in Ω, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega ((u-k)^+)^2 \,\mathrm{d}\mathbf{x} + \int_\Omega |\nabla (u-k)^+|^2 \,\mathrm{d}\mathbf{x}$$
$$= -\int_\Gamma \eta_t (u-k)^+ \,\mathrm{d}s + \frac{1}{2}\int_{\Gamma^{\text{in}}} ((g-k)^+)^2 |\mathbf{V}\cdot\mathbf{v}| \,\mathrm{d}s \leqslant 0$$

because η is a nondecreasing function in t and the integral over Γ^{in} is equal to zero. This implies then the a.e. boundedness of u in Ω_T because of the a.e. boundedness of u_0. Finally, the assertion of the lemma follows from Theorem III.10.1 of [7]. □

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

$$\mathscr{A}_\delta(v)(t) = \begin{cases} 0, & t < \delta \\ \operatorname*{ess\,sup}_{\delta \leqslant s \leqslant t} H(v(s)), & t \geqslant \delta \end{cases}$$

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

$$\gamma_0 \mathscr{A}_\delta(u)(t) = \mathscr{A}_\delta(\gamma_0 u)(t) \quad \text{for all } t \in [0,T] \tag{44}$$

Note that $\mathscr{A}(v)(t) = \|v\|_{L^\infty(0,t)}$ for every nonnegative function $v \in L^\infty(0,T)$, and $\mathscr{A}_\delta(v)(t) = \|\chi_\delta v\|_{L^\infty(0,t)}$, where $\chi_\delta : \mathbb{R} \to \{0,1\}$ is the characteristic function of the interval (δ, T). It is clear that $\mathscr{A}(v)(t) \geqslant \mathscr{A}_\delta(v)(t)$. On the other hand, due to the *-weak semi-continuity of the norm in L^∞, $\mathscr{A}(v)(t) \leqslant \liminf_{\delta \to 0} \mathscr{A}_\delta(v)(t)$. This means that

$$\mathscr{A}(v)(t) = \lim_{\delta \to 0} \mathscr{A}_\delta(v)(t) \tag{45}$$

for almost all $t \in [0,T]$ and for every nonnegative function $v \in L^\infty(0,T)$.

Since the function u is bounded, relation (45) enables us to conclude that

$$\begin{aligned} \mathscr{A}_\delta(u) &\to \mathscr{A}(u) \quad \text{in } L^p(\Omega_T), \, p < \infty \\ \mathscr{A}_\delta(\gamma_0 u) &\to \mathscr{A}(\gamma_0 u) \quad \text{in } L^p(\Gamma_T), \, p < \infty \end{aligned} \tag{46}$$

Lemma 2.11
There exists a constant C_* such that

$$\|\mathscr{A}_\delta(u)\|_{L^\infty(0,T;H^1(\Omega))}\leqslant C_*$$

for every $\delta\geqslant 0$.

Proof
Let us introduce a function q defined on $\partial\Omega$ such that $q=\eta_t$ on Γ and $q=0$ on $\partial\Omega\setminus\Gamma$. Note that $q\geqslant 0$. Consider the problem

$$v_t=\Delta v-\mathbf{V}\cdot\nabla v \quad (\Omega\times(\delta,T)), \quad \frac{\partial v}{\partial \mathbf{v}}=-q \quad (\partial\Omega), \quad v(\mathbf{x},\delta)=u(\mathbf{x},\delta) \tag{47}$$

The solution of this problem is unique so that $v=u$ in $\Omega\times(\delta,T)$. Approximate problem (47) by the following scheme. For every $N\in\mathbb{N}$, set $\tau=(T-\delta)/N$ and consider the problem

$$\begin{aligned}
&v^n-v^{n-1}=\tau\Delta v^n-\tau\mathbf{V}\cdot\nabla v^n, \quad \mathbf{x}\in\Omega\\
&\frac{\partial v^n}{\partial \mathbf{v}}=\begin{cases}-\dfrac{1}{\tau}(\eta(\delta+n\tau)-\eta(\delta+(n-1)\tau)), & \mathbf{x}\in\Gamma\\ 0, & \mathbf{x}\in\partial\Omega\setminus\Gamma\end{cases}\\
&v^0(\mathbf{x})=u(\mathbf{x},\delta)
\end{aligned}$$

Since $\nabla u(\cdot,\delta)\in L^2(\Omega)$ for almost all $\delta\in(0,T)$, this problem is absolutely similar to that given by (15)–(17). Therefore, the function $v_N(\mathbf{x},t)$ and $\bar{v}_N(\mathbf{x},t)$, the piecewise linear and piecewise constant time interpolations of $\{v^n(\mathbf{x})\}$, satisfy the same estimates as $u_N(\mathbf{x},t)$ and $\bar{u}_N(\mathbf{x},t)$. Application of Lemmas 2.5 and 2.7 yields:

$$\|\mathscr{A}_\delta(\bar{v}_N)\|^2_{L^\infty(0,T;H^1(\Omega))}\leqslant\max\{\|H(u^0)\|^2_{L^\infty(\Omega)},\|H(g)\|^2_{L^\infty(\Gamma^{\text{in}};|\mathbf{V}\cdot\mathbf{v}|\,ds)}\}+c_0^2B=:C_*^2$$

and the passage to the limit as $N\to\infty$ implies the estimate

$$\|\mathscr{A}_\delta(v)\|_{L^\infty(0,T;H^1(\Omega))}\leqslant C_*$$

for almost all $\delta\in(0,T)$ and, consequently, for all δ because the definition of $\mathscr{A}_\delta$ utilizes the essential supremum. The equality $\mathscr{A}_\delta(v)=\mathscr{A}_\delta(u)$ proves the Lemma. □

Lemma 2.11 implies that every sequence δ_k that tends to zero as $k\to\infty$ has a subsequence (denoted again by δ_k) such that $\mathscr{A}_{\delta_k}(u)$ converges weakly in $L^2(0,T;H^1(\Omega))$. Owing to the first relation of (46), the limit is equal to $\mathscr{A}(u)$. The uniqueness of the limit for all subsequences $\mathscr{A}_{\delta_k}(u)$ implies that $\mathscr{A}_\delta(u)\to\mathscr{A}(u)$ weakly in $L^2(0,T;H^1(\Omega))$ as $\delta\to 0$. Therefore, $\gamma_0\mathscr{A}_\delta(u)\to\gamma_0\mathscr{A}(u)$ weakly in $L^2(\Gamma_T)$. Finally, due to (44) and the second relation of (46), we conclude that

$$\gamma_0\mathscr{A}_\delta(u)\to\gamma_0\mathscr{A}(u) \quad \text{in } L^2(\Gamma_T) \tag{48}$$

The required relation (43) follows now from (44), (46), and (48). Thus, the solvability of *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 $\tilde{u}=u_1-u_2$, $\tilde{\eta}=\eta_1-\eta_2$. Owing to Hilpert's inequality (see [4, Theorem III.2.6]), it holds that

$$\frac{\mathrm{d}\tilde{\eta}^{+}(\mathbf{x},\cdot)}{\mathrm{d}t}\leqslant\frac{\mathrm{d}\tilde{\eta}(\mathbf{x},\cdot)}{\mathrm{d}t}q(\mathbf{x},\cdot)\quad\text{a.e. in }(0,T) \tag{49}$$

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

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

Multiply (8) by $q_m(\mathbf{x},t)=H_e^m(\tilde{u}(\mathbf{x},t))$, where

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

Since

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

and

$$\nabla H_e^m(\tilde{u}(\mathbf{x},t))\cdot\tilde{u}(\mathbf{x},t)=\frac{1}{m}\nabla H_e^m(\tilde{u}(\mathbf{x},t))\cdot H_e^m(\tilde{u}(\mathbf{x},t))$$

Lemma 2.2 yields

$$\begin{aligned}\int_\Omega \mathbf{V}\cdot\nabla\tilde{u}\cdot H_e^m(\tilde{u})\,\mathrm{d}\mathbf{x}&=\int_{\Gamma^{\text{in}}\cup\Gamma^{\text{out}}}\tilde{u}H_e^m(\tilde{u})(\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s-\frac{1}{m}\int_\Omega \mathbf{V}\cdot\nabla H_e^m(\tilde{u})\cdot H_e^m(\tilde{u})\,\mathrm{d}\mathbf{x}\\&=\int_{\Gamma^{\text{in}}\cup\Gamma^{\text{out}}} H_e^m(\tilde{u})\left[\tilde{u}-\frac{1}{2m}H_e^m(\tilde{u})\right](\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s\end{aligned}$$

Note that $H_e^m(\tilde{u})[\tilde{u}-H_e^m(\tilde{u})/2m]\geqslant 0$. In fact: if $\tilde{u}>0$, then $\tilde{u}\geqslant H_e^m(\tilde{u})/m$ and $H_e^m(\tilde{u})>0$; if $\tilde{u}\leqslant 0$, then $H_e^m(\tilde{u})=0$. Thus, the relation

$$\int_\Omega \frac{\partial\tilde{u}}{\partial t}H_e^m(\tilde{u})\,\mathrm{d}\mathbf{x}+\int_\Gamma \frac{\partial\tilde{\eta}}{\partial t}H_e^m(\tilde{u})\,\mathrm{d}s\leqslant-\int_{\Gamma^{\text{in}}} H_e^m(\tilde{u})\left[\tilde{u}-\frac{1}{2m}H_e^m(\tilde{u})\right](\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s=0$$

holds for almost all $t\in(0,T)$, since $u_1=u_2$ on Γ^{in} and

$$-\int_{\Gamma^{\text{out}}} H_e^m(\tilde{u})\left[\tilde{u}-\frac{1}{2m}H_e^m(\tilde{u})\right](\mathbf{V}\cdot\mathbf{v})\,\mathrm{d}s\leqslant 0$$

due to our assumptions on $\mathbf{V}$. The passage to the limit as $m\to 0$ yields:

$$\int_\Omega \frac{\partial \tilde{u}}{\partial t} q\,\mathrm{d}\mathbf{x}+\int_\Gamma \frac{\partial \tilde{\eta}}{\partial t} q\,\mathrm{d}s\leqslant 0 \quad \text{a.e. in } (0,T)$$

where $q\in H_e(\tilde{u})$ is a function such that $H_e^m(\tilde{u})\to q$ almost everywhere in Γ_T. Using inequality (49) implies:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_\Omega \tilde{u}^+\,\mathrm{d}\mathbf{x}+\int_\Gamma \tilde{\eta}^+\,\mathrm{d}s\right)\leqslant 0$$

This means that $\tilde{u}^+=0$ and $\tilde{\eta}^+=0$. By changing indices 1 and 2, we conclude that $\tilde{u}=0$ and $\tilde{\eta}=0$. The theorem is proved.

3. NUMERICAL COMPUTATIONS

This section describes an approximation of *Problem A* and presents some numerical results. Note that system (8)–(11) is nonlinear with respect to u and η because of conditions (6) and (10). Therefore, fixed-point iteration techniques have to be applied to (8)–(11). Henceforth, equations are formulated in a weak form in space, which assumes numerical treatment of them with the Finite Element Method.

3.1. Time discretization

Consider the same time discretization of (13) as in Section 2.1. Suppose that the functions u^{n-1}, η^{n-1}, and $\mathbf{V}$ are already known at the time instants $t_{n-1}=(n-1)\tau$ and $t_n=n\tau$, respectively. To compute u^n and η^n, use (19) to express η^n in terms of u^n and η^{n-1} and solve the following weak-form problem:

$$\int_\Omega u^n\psi\,\mathrm{d}\mathbf{x}+\tau\int_\Omega [\nabla u^n-u^n\mathbf{V}]\nabla\psi\,\mathrm{d}\mathbf{x}+\int_{\Gamma^{\text{out}}} u^n\psi|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s+\int_\Gamma (H(u^n)-\eta^{n-1})^+\psi\,\mathrm{d}s$$
$$=\int_\Omega u^{n-1}\psi\,\mathrm{d}\mathbf{x}-\tau\int_{\Gamma^{\text{in}}} g\psi|\mathbf{V}\cdot\mathbf{v}|\,\mathrm{d}s \tag{50}$$

Since the term $(H(u^n)-\eta^{n-1})^+$ is nonlinear in u^n, Equation (50) cannot be solved directly, and, therefore, fixed-point iteration techniques should be used here. First, note that

$$(H(u^n)-\eta^{n-1})^+=h(u^n)\cdot(H(u^n)-\eta^{n-1}) \tag{51}$$

where

$$h(u^n)(x)=\begin{cases}0 & \text{if } H(u^n)(x)\leqslant\eta^{n-1}(x)\\ 1 & \text{if } H(u^n)(x)>\eta^{n-1}(x)\end{cases}$$

To obtain a fixed-point iteration scheme for finding u^n, choose a small $c>0$, and write (51) as

$$(H(u^n)-\eta^{n-1})^+ = \left(H(u^n)\frac{u^n+c}{u^n+c}-\eta^{n-1}\right)^+$$
$$= h(u^n)\left[H(u^n)\frac{u^n}{u^n+c}-\left(\eta^{n-1}-H(u^n)\frac{c}{u^n+c}\right)\right] \tag{52}$$

Lemma 2.4 shows that $u^n \geqslant 0$ a.e. in Ω. Therefore, $(u^n+c)^{-1}$ is well defined. Substituting Equation (52) into (50) yields:

$$\int_\Omega u^n \psi \,\mathrm{d}\mathbf{x} + \tau \int_\Omega \nabla u^n \nabla \psi \,\mathrm{d}\mathbf{x} + \int_{\Gamma^{\text{out}}} u^n \psi |\mathbf{V}\cdot\mathbf{v}| \,\mathrm{d}s + \int_\Gamma \frac{h(u^n)H(u^n)}{u^n+c} u^n \psi \,\mathrm{d}s$$
$$= \int_\Omega u^{n-1}\psi \,\mathrm{d}\mathbf{x} - \tau \int_{\Gamma^{\text{in}}} g\psi |\mathbf{V}\cdot\mathbf{v}| \,\mathrm{d}s + \int_\Omega u^n \mathbf{V} \nabla \psi \,\mathrm{d}\mathbf{x} + \int_\Gamma h(u^n)\left(\eta^{n-1} - \frac{cH(u^n)}{u^n+c}\right)\psi \,\mathrm{d}s \tag{53}$$

Compute functions $\tilde{u}^k$ for $k \in \mathbb{N}$ with $\tilde{u}^0 = u^{n-1}$ using the following equation:

$$\int_\Omega \tilde{u}^k \psi \,\mathrm{d}\mathbf{x} + \tau \int_\Omega \nabla \tilde{u}^k \nabla \psi \,\mathrm{d}\mathbf{x} + \int_{\Gamma^{\text{out}}} \tilde{u}^k \psi |\mathbf{V}\cdot\mathbf{v}| \,\mathrm{d}s + \int_\Gamma \frac{h(\tilde{u}^{k-1})H(\tilde{u}^{k-1})}{\tilde{u}^{k-1}+c} \tilde{u}^k \psi \,\mathrm{d}s$$
$$= \int_\Omega u^{n-1}\psi \,\mathrm{d}\mathbf{x} - \tau \int_{\Gamma^{\text{in}}} g\psi |\mathbf{V}\cdot\mathbf{v}| \,\mathrm{d}s + \int_\Omega \tilde{u}^{k-1} \mathbf{V} \nabla \psi \,\mathrm{d}\mathbf{x}$$
$$+ \int_\Gamma h(\tilde{u}^{k-1})\left(\eta^{n-1} - \frac{cH(\tilde{u}^{k-1})}{\tilde{u}^{k-1}+c}\right)\psi \,\mathrm{d}s \tag{54}$$

Note that Equation (54) is obtained from Equation (53) where each appearance of u^n is replaced either by $\tilde{u}^k$ or by $\tilde{u}^{k-1}$ so that the resulting Equation (54) becomes linear with respect to $\tilde{u}^k$. Equation (54) generates a sequence $\{\tilde{u}^k\}_{k=1}^m$ that stops when $\|\tilde{u}^m - \tilde{u}^{m-1}\|_{L^\infty(\Omega)}$ is less than a specified tolerance. Setting $u^n = \tilde{u}^m$ completes the treatment of the nth time step when solving (50).

3.2. Numerical results

The region Ω is chosen as the cube $(0, 0.1)^3$ with Γ^{in} laying in the plane $x_1 = 0$; Γ^{out} in the plane $x_1 = 0.1$; and $\Gamma = \bar{\Omega} \cap \{x_3 = 0\}$. The time-step length τ is equal to 0.003, the number n in the subsequent figures defines the time instants ($t = n\tau$). The initial concentration u^0 of particles is a discontinuous function that assumes constant values in two ellipsoids and is equal to zero outside of them. Three different combinations of the choice of the mass flux g and the velocity $\mathbf{V}$ are considered.

Figure 3 demonstrates numerical results for a closed sensor, which means that $\mathbf{V} = \mathbf{0}$ in Ω and $g = 0$ on Γ^{in}. Since the initial distribution of the particles consists of two ellipsoids, the surface concentration shows two peaks. They grow until the saturation value of η equal to 1 is reached. Simultaneously, the particles spread out over Γ so that the trace $u|_\Gamma$ grows. This causes the rise of the surface concentration around the peaks. The rise stops when the trace $u|_\Gamma$ goes down because of further spreading out the particles.

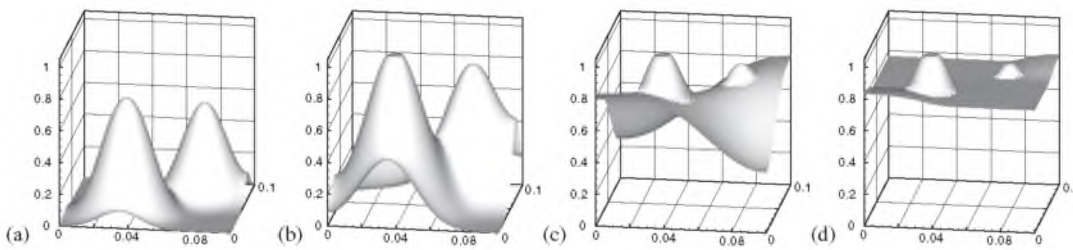

Figure 3. Time snapshots of the surface concentration η in the case $\mathbf{V}=\mathbf{0}$ and $g=0$: (a) $n=15$; (b) $n=45$; (c) $n=345$; and (d) $n=3500$.

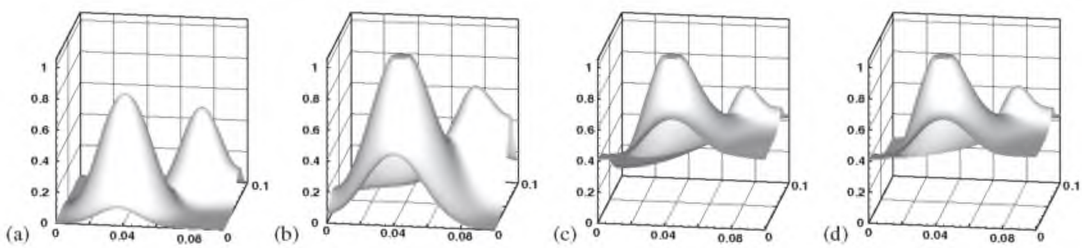

Figure 4. Time snapshots of the surface concentration η in the case $\mathbf{V}=(2,0,0)$ and $g=0$: (a) $n=15$; (b) $n=45$; (c) $n=345$; and (d) $n=3500$.

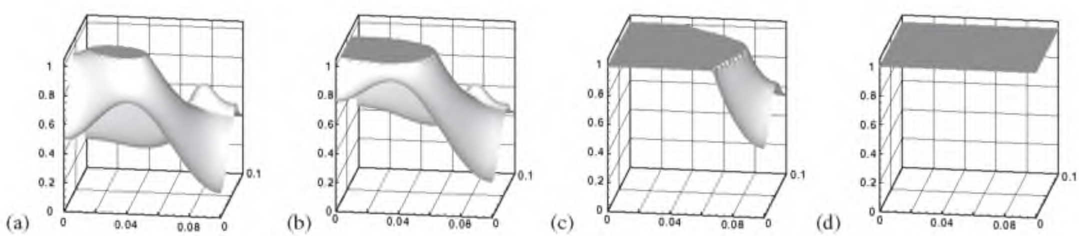

Figure 5. Time snapshots of the surface concentration η in the case $\mathbf{V}=(0.5,0,0)$ and $g=10$: (a) $n=140$; (b) $n=170$; (c) $n=245$; and (d) $n=345$.

Figure 4 shows the results for an open sensor with $\mathbf{V}=(2,0,0)$ on $\Gamma^{in}\cup\Gamma^{out}$ and no incoming particles ($g=0$ on Γ^{in}). Again, two peaks occur because of the initial conditions. Owing to the transport of particles, they are translated in the x_1-direction toward the outlet so that the surface concentration around the peaks increases with x_1.

Figure 5 presents the simulation results for an open sensor with $\mathbf{V}=(2,0,0)$ on $\Gamma^{in}\cup\Gamma^{out}$ and with incoming particles ($g=10$ on Γ^{in}). The development of the surface concentration is similar to that in the case where $g=0$ on the inlet. The difference is that the injection of particles through the inlet results in the uniform saturation of the surface concentration, when time is sufficiently large.

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