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On the existence of a solution for an adsorption dynamic model with the Langmuir isotherm

J. R. FERNÁNDEZ[1], M. C. MUÑIZ[2] and C. NÚÑEZ[3]

[1]*Departamento de Matemática Aplicada I, Universidade de Vigo, ETSI Telecomunicación, Campus As Lagoas Marcosende s/n, 36310 Vigo, Spain*
email: jose.fernandez@uvigo.es
[2]*Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, Facultade de Matemáticas, Campus Vida s/n, 15782 Santiago de Compostela, Spain*
email: mcarmen.muniz@usc.es
[3]*Departamento de Didáctica de las Ciencias Experimentales, Facultad de Ciencias de la Educación, Campus Norte, 15782 Santiago de Compostela, Spain*
email: cristina.nunez.garcia@usc.es

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In this paper, we study an adsorption model arising in the dynamics of several surfactants at the air-water interface, where the Langmuir isotherm is employed for modelling the time-dependent surface concentration, providing a nonlinear dynamical boundary condition. Existence of a weak solution is proved by using the Rothe method for a semi-discrete problem in time. After obtaining some *a priori* estimates and passing to the limit in the time discretization parameter, we conclude that the original Langmuir problem has a bounded solution. An uniqueness result is also given.

Key words: 76T10, 76A20, 76M20, 76M30, 92C45

1 Introduction

Here we focus on the diffusion-controlled model arising in the surfactant behaviour at the air-water interface, using the so-called Langmuir isotherm and a finite diffusion length, as it has been addressed in [2, 16], and has huge applications in the chemical industry (see, for instance, [5, 6, 13] and the references therein). Diffusion is the mechanism that mainly governs this dynamic process since adsorption is assumed to be instantaneous and prescribed by the Langmuir isotherm, which defines a nonlinear relationship between the surface and subsurface concentrations.

From the mathematical point of view, this process is modelled by the diffusion partial differential equation in one spatial dimension, coupled with the Langmuir isotherm by means of a boundary condition at the subsurface, the unknowns being both the bulk and the surface concentrations. This adsorption model yields a non-standard parabolic problem in terms of a nonlinear dynamical boundary condition for which an existence result is provided here. Uniqueness is also proved using a technique previously introduced in [11] for the process of washing contaminants.

Several mathematical investigations have been carried out concerning the different models involved in this problem. The analysis of the problem taking into account the linear Henry isotherm was earlier considered in [9] for the diffusive model and in [10] for the mixed-kinetic one. The mathematical and numerical analyses of the Langmuir–Hinshelwood model for the mixed-kinetic adsorption model are provided in [8]. Moreover, several numerical methods have been used in order to approximate their solutions (see [14, 15] and the references therein). The new contribution of our work is to prove an existence result for the diffusive model including the derivative of the Langmuir isotherm into the boundary condition at the subsurface. We also prove that this solution makes sense from the chemical point of view since it is bounded between zero and the so-called bulk concentration.

The outline of this paper is as follows. In Section 2, we describe the mathematical model and we introduce the variational formulation of the problem. The existence of a bounded weak solution is proved in Section 3 by using the Rothe method, an intermediate problem (for which the existence of a unique weak solution is obtained applying Brouwer's fixed-point theorem), *a priori* estimates and passing to the limit. The uniqueness issue is solved using some arguments already introduced in [11], as the integration in time of the respective variational equations and the definition of adequate test functions.

2 The mathematical model and the variational formulation

In this section we introduce the mathematical framework arising in the modeling of several surfactants at the air-water interface. Indeed, when a new air-water interface is formed, the surfactant molecules tend to migrate onto the interface in order to reduce its surface tension. The analysis of the dynamic surface tension is then closely related to molecular transport, assuming here a lattice-type model where the surfactant surface molecules do not interact with their lattice neighbours or with the vacant sites. Hereafter we refer the bulk as the spatial interval $[0, l]$ occupied by the surfactant, the subsurface being located at $x = 0$ (see [9] for further details). Denoting the concentration of surfactant, at time $t \in [0, T]$ and point $x \in [0, l]$, by $\tilde{c}(t, x)$, and the time-dependent surface concentration by $\Gamma(t)$ and taking into account the Fick's law, we consider the diffusion partial differential equation:

$$\frac{\partial \tilde{c}}{\partial t}(t, x) - D\,\frac{\partial^2 \tilde{c}}{\partial x^2}(t, x) = 0, \quad t > 0, \quad x \in (0, l), \tag{2.1}$$

together with the boundary conditions (see [2]):

$$D\,\frac{\partial \tilde{c}}{\partial x}(t, 0) = \frac{d\Gamma}{dt}(t), \quad t > 0, \tag{2.2}$$

$$\tilde{c}(t, l) = c_b, \quad t > 0, \tag{2.3}$$

and the initial conditions:

$$\tilde{c}(0, x) = \tilde{c}_0(x), \quad x \in (0, l), \tag{2.4}$$

$$\Gamma(0) = \Gamma_0. \tag{2.5}$$

In equations (2.1)–(2.3), D is the diffusion coefficient and the positive constant c_b is the bulk concentration. Besides, in equation (2.4), $\tilde{c}_0(x)$ is a function defined in $[0, l]$ which

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equals c_b on $x = l$, and Γ_0 in equation (2.5) stands for the initial surface concentration, being zero for a fresh surface. We remind the reader that the time-dependent surface concentration, $\Gamma(t)$, is also an unknown of the system, so an additional condition is needed in order to close the problem. As we said previously, we consider the well-known and classical Langmuir isotherm (see [2]):

$$\Gamma(t) = \Gamma_m \frac{K_L\,\tilde{c}(t,0)}{1 + K_L\,\tilde{c}(t,0)}, \quad t \geqslant 0, \tag{2.6}$$

where Γ_m is the maximum surface concentration and K_L is the Langmuir equilibrium adsorption constant. Note also that boundary condition (2.2) together with (2.6) involve the time derivative of the solution at the boundary, introducing then a dynamical boundary condition. Notice that from (2.4)–(2.6) the following compatibility condition is needed:

$$\Gamma_0 = \Gamma_m \frac{K_L\,\tilde{c}_0(0)}{1 + K_L\,\tilde{c}_0(0)}.$$

For the sake of clarity in the presentation and without loss of generality, hereinafter we assume that the constants D, K_L and Γ_m are equal to 1 and we define the nondecreasing Lipschitz function $F : \mathbb{R} \to \mathbb{R}$ as follows

$$F(z) = \begin{cases} \dfrac{z}{1+z} & \text{if } z \geqslant 0, \\ 0 & \text{if } z < 0. \end{cases} \tag{2.7}$$

Notice that a primitive to F given by

$$H(z) = \begin{cases} z - \ln(1+z) & \text{if } z \geqslant 0, \\ 0 & \text{if } z < 0, \end{cases} \tag{2.8}$$

is nondecreasing and convex. Therefore, using (2.7), boundary condition (2.2) can be written as

$$D\frac{\partial \tilde{c}}{\partial x}(t,0) = \frac{d(F \circ \tilde{c}(t,0))}{dt}, \quad t > 0. \tag{2.9}$$

We remark that equation (2.9) determines a nonlinear dynamical boundary condition due to the function F coming from Langmuir isotherm (see [12, 20] and the references therein).

Now, in order to obtain a homogeneous boundary condition in the bulk and simplify the calculations, we define a new variable $c = \tilde{c} - c_b$ and then problem (2.1), (2.3)–(2.5) and (2.9) can be written as follows:

$$\frac{\partial c}{\partial t}(t,x) - \frac{\partial^2 c}{\partial x^2}(t,x) = 0, \quad t > 0, \quad x \in (0,l), \tag{2.10}$$

$$\frac{\partial c}{\partial x}(t,0) = \frac{d(F \circ (c(t,0) + c_b))}{dt}, \quad t > 0, \tag{2.11}$$

$$c(t,l) = 0, \quad t > 0, \tag{2.12}$$

$$c(0,x) = c_0(x), \quad x \in (0,l), \tag{2.13}$$

where $c_0(x) = \tilde{c}_0(x) - c_b$.

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We now obtain the variational formulation of problem (2.10)–(2.13). We write $H = L^2(0,l)$, with $(\cdot,\cdot)_H$ and $\|\cdot\|_H$ its scalar product and its corresponding norm, respectively, defined by (see [1]):

$$(v,w)_H = \int_0^l v(x)\,w(x)\,dx, \quad \|v\|_H = (v,v)_H^{1/2}, \quad \forall v,w,\in H.$$

Moreover, let V be the closed subspace of $H^1(0,l)$ given by

$$V = \{v \in H^1(0,l)\,;\, v(l) = 0\}.$$

On this space V we consider the inner product and the corresponding norm given by

$$((v,w)) = \int_0^l \frac{\partial v}{\partial x}(x)\frac{\partial w}{\partial x}(x)\,dx, \quad \|v\|_V = ((v,v))^{1/2}, \quad \forall v,w \in V.$$

Note that $\|\cdot\|_{H^1(0,l)}$ and $\|\cdot\|_V$ are equivalent norms and so there exists a positive constant C_e such that

$$\|v\|_{H^1(0,l)} \leqslant C_e\|v\|_V, \quad \forall v \in V. \tag{2.14}$$

As usual, we denote the dual space to V by V' and the duality pairing of V and V' by $\langle\cdot,\cdot\rangle_{V'\times V}$. In what follows, we use the space $\mathscr{V} = L^2(0,T;V)$ and

$$\mathscr{W}(0,T) = \left\{v \in \mathscr{V}\,;\, \frac{\partial v}{\partial t} \in \mathscr{V}'\right\}.$$

It is well known (see [19]) that $\mathscr{W}(0,T) \subset \mathscr{V} \subset L^2(0,T;H) \subset \mathscr{V}'$ and $\mathscr{W}(0,T) \subset \mathscr{C}([0,T];H)$. Finally, we denote by $\gamma_0 : H^1(0,l) \to \mathbb{R}$ the trace operator given by $\gamma_0(v) = v(0)$. From the continuity of the trace operator, it follows that

$$|\gamma_0(v)| \leqslant C_{tr}\|v\|_V, \tag{2.15}$$

for all $v \in V$ with $C_{tr} = \|\gamma_0\|_{\mathscr{L}(V,\mathbb{R})}$. Moreover, we assume the following hypothesis:
(H1). The initial condition c_0 belongs to V and $-\mathfrak{C} \leqslant c_0 \leqslant 0$ a.e. in $(0,l)$, where $\mathfrak{C}$ is a positive constant.

Now, assume that c is a smooth function which solves problem (2.10)–(2.13) and let v be a smooth function such that $v(t,l) = 0$ a.e. $t \in (0,T)$. Multiplying equation (2.10) by v, integrating in $(0,l)$ and using integration by parts, we obtain

$$\int_0^l \frac{\partial c}{\partial t}(t,x)v(t,x)dx + \int_0^l \frac{\partial c}{\partial x}(t,x)\frac{\partial v}{\partial x}(t,x)dx + \frac{\partial c}{\partial x}(t,0)v(t,0) = 0,$$

for a.e. $t \in (0,T)$. Using equation (2.11), we find that

$$\int_0^l \frac{\partial c}{\partial t}(t,x)v(t,x)dx + \int_0^l \frac{\partial c}{\partial x}(t,x)\frac{\partial v}{\partial x}(t,x)dx + \frac{d(F\circ(c(t,0)+c_b))}{dt}v(t,0) = 0, \tag{2.16}$$

for a.e. $t \in (0,T)$. Integrating now in $(0,T)$, we have the following weak formulation of problem (2.10)–(2.13).

Problem P_W. For a given $c_0 \in H$, find a function $c \in \mathscr{W}(0,T)$ such that $F(\gamma_0(c(t))+c_b) \in H^1(0,T)$, and

$$\int_0^T \left\langle \frac{\partial c}{\partial t}(t), v(t) \right\rangle_{V' \times V} dt + \int_0^T ((c(t), v(t)))dt$$

$$+ \int_0^T \frac{d(F(\gamma_0(c(t))+c_b))}{dt} \gamma_0(v(t))\, dt = 0, \quad \forall v \in \mathscr{V}, \tag{2.17}$$

$$c(0) = c_0. \tag{2.18}$$

We remark that the initial condition (2.18) makes sense since the inclusion $\mathscr{W}(0,T) \subset \mathscr{C}([0,T];H)$ is satisfied.

3 Existence and uniqueness results

In this section, we use the Rothe method of semi-discretization in time (see [18]) in order to prove the existence of solution to Problem P_W. The scheme of the proof is as follows: the first step is to consider the semi-discretization in time of problem (2.16) and show that this problem has a unique solution; secondly, using this solution, we construct piecewise constant and piecewise linear in time functions and then, using some estimates of these functions and passing to the limit, we arrive at the existence result.

First of all, before dealing with the proof of existence, we introduce the following technical lemma gathering the properties of functions F and H that will be useful later.

Lemma 1 *Functions F and H, defined in (2.7) and (2.8), respectively, satisfy the following properties:*

$$F(z)z - H(z) \geqslant 0, \quad \forall z \in \mathbb{R}, \tag{3.1}$$

$$(F(z_1) - F(z_2))(z_1 - z_2) \geqslant (F(z_1) - F(z_2))^2, \quad \forall z_1, z_2 \in \mathbb{R}. \tag{3.2}$$

Proof Taking into account the definitions of functions F and H given by (2.7) and (2.8), respectively, (3.1) is trivially obtained for $z < 0$. Otherwise, if z is nonnegative, we define the function

$$G(z) = F(z)z - H(z),$$

and then, we have $G(0) = 0$ and $G \in \mathscr{C}^1([0,\infty)]$. Moreover, for $z \geqslant 0$, $G'(z) = \frac{z}{(1+z)^2} \geqslant 0$ and, therefore, $G(z) \geqslant G(0) = 0$.

Thus, property (3.1) follows. Now, taking into account that F is nondecreasing and 1-Lipschitz, it follows that, for all $z_1, z_2 \in \mathbb{R}$,

$$(F(z_1) - F(z_2))(z_1 - z_2) = |F(z_1) - F(z_2)|\,|z_1 - z_2| \geqslant (F(z_1) - F(z_2))^2,$$

and property (3.2) is obtained. □

Now, we prove the following preliminary result.

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Lemma 2 *Assuming that $c_{s-1} \in V$ and $\tau > 0$, there exists a unique function $c_s \in V$ such that, for all $v \in V$,*

$$\int_0^l \frac{(c_s - c_{s-1})}{\tau} v dx + \frac{F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b)}{\tau} \gamma_0(v) + \int_0^l \frac{\partial c_s}{\partial x} \frac{\partial v}{\partial x} dx = 0. \quad (3.3)$$

Moreover, if $-\mathfrak{C} \leqslant c_{s-1} \leqslant 0$ a.e. in $(0,l)$ then

$$-\mathfrak{C} \leqslant c_s \leqslant 0 \text{ a.e. in } (0,l), \quad (3.4)$$

$\mathfrak{C}$ being a positive constant.

Proof *Existence.* The proof of the existence of a solution to the nonlinear problem (3.3) is based on the study of an intermediate problem, followed by the application of Brouwer's fixed point theorem (see [7]).

Intermediate problem. For a given $c_{s-1} \in V$, $\tau > 0$ and $c^\star \in \mathbb{R}$, find $c \in V$ such that, for all $v \in V$,

$$\int_0^l \frac{(c - c_{s-1})}{\tau} v dx + \frac{F(c^\star + c_b) - F(\gamma_0(c_{s-1}) + c_b)}{\tau} \gamma_0(v) + \int_0^l \frac{\partial c}{\partial x} \frac{\partial v}{\partial x} dx = 0. \quad (3.5)$$

The existence of a unique solution to problem (3.5) can be straightforwardly proved applying the Lax-Milgram theorem, by taking into account that the bilinear mapping

$$a(u,v) = \int_0^l u v dx + \tau \int_0^l \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} dx$$

is continuous and coercive in V, and the functional

$$L(v) = \int_0^l c_{s-1} v dx + (F(\gamma_0(c_{s-1}) + c_b) - F(c^\star + c_b)) \gamma_0(v)$$

belongs to V'.

Now, we define the operator $G : \mathbb{R} \to \mathbb{R}$ given by $G(c^\star) = \gamma_0(c)$, where $c \in V$ is the unique solution to problem (3.5) corresponding to $c^\star$. Moreover, for the operator G, we find that G maps $[-M, M]$ into itself, where

$$M := \frac{C_{tr}\, C_e \|c_{s-1}\|_H + C_{tr}^2}{\tau},$$

C_{tr} and C_e being the trace constant and the norms equivalence constant (see (2.15) and (2.14), respectively).

Indeed, in order to prove that G maps $[-M, M]$ into itself, we take $c \in V$ as a test function in (3.5) and we get

$$\int_0^l c^2 dx + \int_0^l \tau \left(\frac{\partial c}{\partial x}\right)^2 dx = \int_0^l c_{s-1}\, c\, dx + (F(\gamma_0(c_{s-1}) + c_b) - F(c^\star + c_b))\gamma_0(c).$$

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Using the Hölder and trace inequalities and the fact that $|F(a)-F(b)| \leqslant 1$, for all $a, b \in \mathbb{R}$, and taking into account that the first term of the previous equality is nonnegative and (2.14), we have

$$\tau\|c\|_V^2 \leqslant C_e\|c_{s-1}\|_H\|c\|_V + C_{tr}\|c\|_V.$$

Now, dividing by $\|c\|_V$ and using the trace inequality again, we obtain

$$|\gamma_0(c)| \leqslant C_{tr}\frac{C_e\|c_{s-1}\|_H + C_{tr}}{\tau} = M.$$

In order to be able to apply Brouwer's fixed point theorem, we have to show that G is a continuous operator. For that purpose, let us consider $\{c_m^\star\}_{m\in\mathbb{N}} \subset \mathbb{R}$ such that $\{c_m^\star\}_{m\in\mathbb{N}} \to c^\star$ in $\mathbb{R}$ and, for each $c_m^\star, m \in \mathbb{N}$, let c_m be the solution to the problem:

$$\int_0^l \frac{(c_m - c_{s-1})}{\tau} v dx + \frac{F(c_m^\star + c_b) - F(\gamma_0(c_{s-1}) + c_b)}{\tau}\gamma_0(v) + \int_0^l \frac{\partial c_m}{\partial x}\frac{\partial v}{\partial x}dx = 0, \quad \forall v \in V. \tag{3.6}$$

Subtracting (3.6) and (3.5) and taking $v = c_m - c \in V$ as a test function, we get

$$\int_0^l (c_m - c)^2\, dx + \tau\int_0^l \left(\frac{\partial(c_m - c)}{\partial x}\right)^2 dx = (F(c^\star + c_b) - F(c_m^\star + c_b))\gamma_0(c_m - c).$$

Since the first term of the previous equality is nonnegative, it follows that

$$\tau\|c_m - c\|_V^2 \leqslant |F(c_m^\star + c_b) - F(c^\star + c_b)|\,|\gamma_0(c_m - c)|.$$

Using the trace inequality (2.15) we obtain

$$\frac{\tau}{C_{tr}^2}|\gamma_0(c_m - c)|^2 \leqslant |F(c_m^\star + c_b) - F(c^\star + c_b)|\,|\gamma_0(c_m - c)|.$$

Finally, taking into account that F is 1-Lipschitz, we have

$$|\gamma_0(c_m - c)| \leqslant \frac{C_{tr}^2}{\tau}|c_m^\star - c^\star|.$$

Since $|c_m^\star - c^\star| \to 0$ we get the continuity of G. Therefore, Brouwer's fixed-point theorem guarantees the existence of a fixed point of G, i.e. there exists an element $c^\star \in [-M, M]$ such that $G(c^\star) = c^\star$ and the result follows.

Uniqueness. Let us assume that there exist two solutions, c_s^1 and c_s^2, to problem (3.3). We subtract the resulting two equations obtained for $c_s = c_s^1$ and $c_s = c_s^2$, respectively, and take $v = c_s^1 - c_s^2 \in V$ as a test function, then

$$\int_0^l \left(c_s^1 - c_s^2\right)^2 dx + \tau\int_0^l \left(\frac{\partial\left(c_s^1 - c_s^2\right)}{\partial x}\right)^2 dx + (F\left(\gamma_0\left(c_s^1\right) + c_b\right) - F\left(\gamma_0\left(c_s^2\right) + c_b\right))\gamma_0\left(c_s^1 - c_s^2\right) = 0. \tag{3.7}$$

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Since F is nondecreasing, all terms in the left-hand side are nonnegative. Therefore, we can conclude from (3.7) that all its terms are equal to zero, and then $c_s^1(x) = c_s^2(x)$ for $x \in (0,l)$.

In order to prove (3.4), we take $v = c_s^+ = \max\{c_s, 0\} \in V$ as a test function in (3.3) to get

$$\int_0^l (c_s^+)^2\,dx + (F(\gamma_0(c_s)+c_b) - F(\gamma_0(c_{s-1})+c_b))\gamma_0(c_s^+) + \tau \int_0^l \left(\frac{\partial c_s^+}{\partial x}\right)^2 dx$$
$$= \int_0^l c_{s-1}\, c_s^+ dx.$$

Notice that, if $\gamma_0(c_s^+) = 0$, then the second term of the previous equation disappears. On the contrary, if $\gamma_0(c_s^+)$ is positive then $\gamma_0(c_s)$ is positive. Moreover, since $c_{s-1} \leqslant 0$ a.e. in $(0,l)$ and $c_{s-1} \in V \subset \mathscr{C}([0,l])$ (see [17]), it follows that $\gamma_0(c_{s-1}) \leqslant 0$. Then, due to the nondecreasing behaviour of function F we know that $F(\gamma_0(c_s)+c_b) - F(\gamma_0(c_{s-1})+c_b) \geqslant 0$. Therefore, in both cases, the left-hand side of the previous equality is nonnegative, while the right-hand side is nonpositive and we can conclude that $c_s^+ = 0$ a.e. in $(0,l)$. Thus $c_s \leqslant 0$ a.e. in $(0,l)$.

Finally, we take $v = (c_s + \mathfrak{C})^- = \max\{0, -(c_s + \mathfrak{C})\} \in H^1(0,l)$. Notice that $v(l) = \max\{0, -(c_s(l) + \mathfrak{C})\} = \max\{0, -\mathfrak{C}\} = 0$, then $v \in V$ and it can be taken as a test function in equation (3.3) to obtain

$$\int_0^l (c_s - c_{s-1})(c_s + \mathfrak{C})^- dx + (F(\gamma_0(c_s)+c_b) - F(\gamma_0(c_{s-1})+c_b))\gamma_0(c_s+\mathfrak{C})^-$$
$$-\tau \int_0^l \left(\frac{\partial (c_s+\mathfrak{C})^-}{\partial x}\right)^2 dx = 0. \tag{3.8}$$

By using the hypothesis $-\mathfrak{C} \leqslant c_{s-1}$ in $(0,l)$ we have

$$\int_0^l (c_s - c_{s-1})(c_s + \mathfrak{C})^- dx = \int_{[c_s \leqslant -\mathfrak{C}]} (c_s - c_{s-1})(c_s + \mathfrak{C})^- dx \leqslant 0.$$

Moreover, if $\gamma_0(c_s) < -\mathfrak{C}$, then $\gamma_0(c_s + \mathfrak{C})^- > 0$ and $\gamma_0(c_s) < \gamma_0(c_{s-1})$. Taking into account that F is nondecreasing we get $F(\gamma_0(c_s)+c_b) \leqslant F(\gamma_0(c_{s-1})+c_b)$. Hence, all terms in equation (3.8) are nonpositive and then $(c_s + \mathfrak{C})^- = 0$ a.e. in $(0,l)$ and, consequently, $-\mathfrak{C} \leqslant c_s$ a.e. in $(0,l)$. □

Now, regarding c_s as the solution to problem (3.3) at time $t = s$ we define the following piecewise constant and piecewise linear in time functions.

Definition 3.1 Assuming that $c_0 \in V$, let c_s be the solution to problem (3.3) at time $t = s$, $s \in \mathbb{N}$. Then, for $(0,T] = \bigcup_{s=1}^K ((s-1)\tau, s\tau]$, with $\tau = T/K$ and $K \in \mathbb{N}$, we define the piecewise linear and piecewise constant in time functions

$$\tilde{c}_\tau,\ c_\tau : [0,T] \to V$$

given by

$$\tilde{c}_\tau(t,x) := c_s(x), \tag{3.9}$$

$$c_\tau(t,x) := \left(s - \frac{t}{\tau}\right) c_{s-1}(x) + \left(\frac{t}{\tau} - s + 1\right) c_s(x), \tag{3.10}$$

for $x \in (0,l)$ and $(s-1)\tau \leqslant t < s\tau$, $s = 1,\dots,K$. Moreover, we define $F_\tau : [0,T] \to \mathbb{R}$ as follows:

$$F_\tau(t) := \left(s - \frac{t}{\tau}\right) F(\gamma_0(c_{s-1}) + c_b) + \left(\frac{t}{\tau} - s + 1\right) F(\gamma_0(c_s) + c_b), \tag{3.11}$$

for $(s-1)\tau \leqslant t < s\tau$, $s = 1,\dots,K$.

Remark 1 *Note that*

$$\frac{\partial c_\tau}{\partial t}(t,x) = \frac{c_s(x) - c_{s-1}(x)}{\tau}, \tag{3.12}$$

$$\frac{dF_\tau}{dt}(t) = \frac{F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b)}{\tau}, \tag{3.13}$$

for $x \in (0,l)$ and $(s-1)\tau < t < s\tau$, $s = 1,\dots,K$, and problem (3.3) can be written for a.e. $t \in (0,T)$ in the form

$$\int_0^l \frac{\partial c_\tau}{\partial t} v\,dx + \frac{dF_\tau}{dt}\gamma_0(v) + \int_0^l \frac{\partial \tilde{c}_\tau}{\partial x}\frac{\partial v}{\partial x}\,dx = 0, \quad \forall v \in V. \tag{3.14}$$

Note also that

$$c_\tau - \tilde{c}_\tau = \left(\frac{t}{\tau} - s\right)(c_s - c_{s-1}) = \left(\frac{t}{\tau} - s\right)\tau\,\frac{\partial c_\tau}{\partial t}, \tag{3.15}$$

for $x \in (0,l)$ and $(s-1)\tau < t < s\tau$, $s = 1,\dots,K$.

Definition 3.2 Regarding the functions F and H defined in (2.7) and (2.8), respectively, for $s = 1,\dots,K$, we define

$$M_s := \int_0^l \frac{c_s^2}{2}dx + F(\gamma_0(c_s) + c_b)(\gamma_0(c_s) + c_b) - H(\gamma_0(c_s) + c_b),$$

and

$$N_s := c_b F(\gamma_0(c_s) + c_b).$$

We have the following energy decay property.

Lemma 3 *Assuming that $c_0 \in V$, it follows that*

$$M_s + \tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant M_{s-1} + c_b,\ s = 1,\dots,K, \tag{3.16}$$

$$M_K - N_K \leqslant \cdots \leqslant M_s - N_s \leqslant M_{s-1} - N_{s-1} \leqslant \cdots \leqslant M_0 - N_0, \tag{3.17}$$

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where $c_s \in V$, $s = 1,\ldots,K$, are the solutions to problem (3.3). Moreover,

$$\sum_{n=1}^{s} \tau \int_0^l \left(\frac{\partial c_n}{\partial x}\right)^2 dx \leqslant M_0 + c_b, \; s = 1,\ldots,K, \tag{3.18}$$

and

$$M_s \leqslant M_0 + c_b, \; s = 1,\ldots,K. \tag{3.19}$$

Proof Taking $v = c_s$ as a test function in problem (3.3), we get, for $s = 1,\ldots,K$,

$$\int_0^l (c_s - c_{s-1})c_s \, dx + (F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))\gamma_0(c_s) + \tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx = 0.$$

Furthermore, using the fact that $x(x-y) \geqslant (x^2 - y^2)/2$, for $x, y \in \mathbb{R}$, in the first term of the latter expression, we have, for $s = 1,\ldots,K$,

$$\int_0^l \frac{c_s^2}{2} dx - \int_0^l \frac{c_{s-1}^2}{2} dx + (F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))(\gamma_0(c_s) + c_b - c_b)$$
$$+\tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant 0. \tag{3.20}$$

Keeping in mind that

$$\begin{aligned}(F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))(\gamma_0(c_s) + c_b) &= F(\gamma_0(c_s) + c_b)(\gamma_0(c_s) + c_b) \\ &\quad -F(\gamma_0(c_{s-1}) + c_b)(\gamma_0(c_{s-1}) + c_b) \\ &\quad +F(\gamma_0(c_{s-1}) + c_b)\big((\gamma_0(c_{s-1}) + c_b) - (\gamma_0(c_s) + c_b)\big),\end{aligned} \tag{3.21}$$

and, since the primitive H of F, defined in (2.8), is convex, we get (see [7])

$$H(\gamma_0(c_{s-1}) + c_b) - H(\gamma_0(c_s) + c_b) \leqslant F(\gamma_0(c_{s-1}) + c_b)(\gamma_0(c_{s-1}) - \gamma_0(c_s)). \tag{3.22}$$

Taking into account (3.21) and (3.22) in (3.20), we obtain, for $s = 1,\ldots,K$,

$$\int_0^l \frac{c_s^2}{2} dx - \int_0^l \frac{c_{s-1}^2}{2} dx + F(\gamma_0(c_s) + c_b)(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b)(\gamma_0(c_{s-1}) + c_b)$$
$$+H(\gamma_0(c_{s-1}) + c_b) - H(\gamma_0(c_s) + c_b) - c_b F(\gamma_0(c_s) + c_b) + c_b F(\gamma_0(c_{s-1}) + c_b)$$
$$+\tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant 0.$$

Therefore, it follows that, for $s = 1,\ldots,K$,

$$M_s - M_{s-1} - N_s + N_{s-1} + \tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant 0, \tag{3.23}$$

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and we find that, for $s = 1, \dots, K$,

$$M_s + \tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant M_{s-1} - N_{s-1} + N_s. \tag{3.24}$$

We remark here that, since we have $F(z) \in [0,1)$ for all $z \in \mathbb{R}$, we get $0 \leqslant N_s < c_b$, for $s = 1, \dots, K$, and, from (3.24), we conclude that

$$M_s + \tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant M_{s-1} + N_s \leqslant M_{s-1} + c_b, \qquad s = 1, \dots, K. \tag{3.25}$$

Thus, (3.16) holds. Moreover, from (3.23) and taking into account that its fifth term is nonnegative, we get

$$M_s - N_s \leqslant M_{s-1} - N_{s-1}, \qquad s = 1, \dots, K,$$

and (3.17) holds. Also, from (3.23) we have

$$M_s - N_s + \tau \int_0^l \left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant M_{s-1} - N_{s-1}, \qquad s = 1, \dots, K,$$

and adding the term $\tau \sum_{n=1}^{s-1} \int_0^l (\frac{\partial c_n}{\partial x})^2 dx$ to both sides of the latter inequality, it follows that

$$M_s - N_s + \tau \sum_{n=1}^{s} \int_0^l \left(\frac{\partial c_n}{\partial x}\right)^2 dx \leqslant M_0 - N_0, \qquad s = 1, \dots, K.$$

Finally, considering that $N_s \in [0, c_b], s = 0, \dots, K$, we obtain, for $s = 1, \dots, K$,

$$M_s + \tau \sum_{n=1}^{s} \int_0^l \left(\frac{\partial c_n}{\partial x}\right)^2 dx \leqslant M_0 - N_0 + N_s \leqslant M_0 + N_s \leqslant M_0 + c_b. \tag{3.26}$$

Note that we can guarantee that $M_s \geqslant 0$ taking into account that its first term is nonnegative and using (3.1). Thus, from (3.26) we obtain (3.18) and (3.19). □

We have the following *a priori* estimates.

Proposition 1 *Assuming the hypothesis (H1) with $\mathfrak{C} = c_b$, then functions $\tilde{c}_\tau$ and c_τ, defined in (3.9) and (3.10), respectively, are bounded in the space $L^2(0,T;H^1(0,l))$. Moreover, c_τ is bounded in $H^1(0,T;H)$ and F_τ, defined in (3.11), is bounded in $H^1(0,T)$ independently of τ. Furthermore,*

$$\|c_\tau - \tilde{c}_\tau\|^2_{L^2(0,T;H)} \leqslant C_1 \tau^2, \tag{3.27}$$

$$\|\gamma_0(c_\tau) - \gamma_0(\tilde{c}_\tau)\|^2_{L^2(0,T)} \leqslant C_2 \tau^2, \tag{3.28}$$

where C_1 and C_2 are real positive constants independent of τ.

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Proof First, we prove that $\tilde{c}_\tau$ is bounded in $L^2(0,T;H^1(0,l))$. Indeed, by definition we have

$$\begin{aligned}
\|\tilde{c}_\tau\|^2_{L^2(0,T;H)} &= \int_0^T \|\tilde{c}_\tau(t)\|^2_H dt \\
&= \sum_{s=1}^K \int_{(s-1)\tau}^{s\tau} \left(\int_0^l (\tilde{c}_\tau(t,x))^2 dx\right) dt \\
&= \sum_{s=1}^K \int_{(s-1)\tau}^{s\tau} \left(\int_0^l (c_s(x))^2 dx\right) dt. \qquad (3.29)
\end{aligned}$$

Using property (3.1) and Lemma 3, we know that

$$\int_0^l \frac{(c_s(x))^2}{2} dx \leqslant M_s \leqslant M_0 + c_b, \qquad s = 1,\dots,K,$$

and thus,

$$\int_0^l (c_s(x))^2 dx \leqslant 2(M_0 + c_b), \qquad s = 1,\dots,K. \qquad (3.30)$$

Keeping in mind (3.29) and (3.30), it follows that

$$\|\tilde{c}_\tau\|^2_{L^2(0,T;H)} \leqslant \sum_{s=1}^K \int_{(s-1)\tau}^{s\tau} (2M_0 + 2c_b)\, dt = (2M_0 + 2c_b)\tau K = (2M_0 + 2c_b)T. \qquad (3.31)$$

Moreover, considering inequalities (3.18) and (3.31), we have

$$\begin{aligned}
\|\tilde{c}_\tau\|^2_{L^2(0,T;H^1(0,l))} &= \int_0^T \|\tilde{c}_\tau(t)\|^2_{H^1(0,l)} dt \\
&= \sum_{s=1}^K \int_{(s-1)\tau}^{s\tau} \left(\int_0^l (c_s(x))^2 dx + \int_0^l \left(\frac{\partial c_s}{\partial x}(x)\right)^2 dx\right) dt \\
&\leqslant (2M_0 + 2c_b)T + \sum_{s=1}^K \tau \int_0^l \left(\frac{\partial c_s}{\partial x}(x)\right)^2 dx \\
&\leqslant (2M_0 + 2c_b)T + M_0 + c_b.
\end{aligned}$$

Thus, we can conclude that $\tilde{c}_\tau$ is bounded in $L^2(0,T;H^1(0,l))$ independently of τ. The following step is to show that c_τ is bounded in $L^2(0,T;H^1(0,l))$ as well. Indeed, by definition we get

$$\|c_\tau\|^2_{L^2(0,T;H)} = \int_0^T \|c_\tau(t)\|^2_H dt = \int_0^T \left\| \left(s - \frac{t}{\tau}\right) c_{s-1} + \left(\frac{t}{\tau} - s + 1\right) c_s \right\|^2_H dt.$$

Regarding that $f(x) = \|x\|^2$ is a convex function and for $(s-1)\tau \leqslant t \leqslant s\tau$, $s = 1,\dots,K$,

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we get that $0 \leqslant s - \frac{t}{\tau} < 1$, then

$$\|c_\tau\|^2_{L^2(0,T;H)} \leqslant \int_0^T \left(\left(s - \frac{t}{\tau} \right) \|c_{s-1}\|^2_H + \left(\frac{t}{\tau} - s + 1 \right) \|c_s\|^2_H \right) dt$$
$$= \int_0^T \left(\left(s - \frac{t}{\tau} \right) \int_0^l (c_{s-1}(x))^2 dx + \left(\frac{t}{\tau} - s + 1 \right) \int_0^l (c_s(x))^2 dx \right) dt.$$

Now, using inequality (3.30), we have

$$\|c_\tau\|^2_{L^2(0,T;H)} \leqslant \sum_{s=1}^{K} \int_{(s-1)\tau}^{s\tau} \left(\left(s - \frac{t}{\tau} \right) 2(M_0 + c_b) + \left(\frac{t}{\tau} - s + 1 \right) 2(M_0 + c_b) \right) dt$$
$$= \sum_{s=1}^{K} \int_{(s-1)\tau}^{s\tau} 2(M_0 + c_b)\, dt = 2(M_0 + c_b) \sum_{s=1}^{K} \tau = 2(M_0 + c_b)T.$$

Using the same arguments, we also get

$$\left\| \frac{\partial c_\tau}{\partial x} \right\|^2_{L^2(0,T;H)} = \int_0^T \left\| \frac{\partial c_\tau}{\partial x}(t) \right\|^2_H = \int_0^T \left\| \left(s - \frac{t}{\tau} \right) \frac{\partial c_{s-1}}{\partial x} + \left(\frac{t}{\tau} - s + 1 \right) \frac{\partial c_s}{\partial x} \right\|^2_H dt$$
$$\leqslant \sum_{s=1}^{K} \int_{(s-1)\tau}^{s\tau} \left(\left(s - \frac{t}{\tau} \right) \int_0^l \left(\frac{\partial c_{s-1}}{\partial x}(x) \right)^2 dx + \left(\frac{t}{\tau} - s + 1 \right) \int_0^l \left(\frac{\partial c_s}{\partial x}(x) \right)^2 dx \right) dt$$
$$= \frac{\tau}{2} \int_0^l \left(\frac{\partial c_0}{\partial x}(x) \right)^2 dx + \sum_{s=1}^{K-1} \frac{\tau}{2} \int_0^l \left(\frac{\partial c_s}{\partial x}(x) \right)^2 dx + \sum_{s=1}^{K} \frac{\tau}{2} \int_0^l \left(\frac{\partial c_s}{\partial x}(x) \right)^2 dx,$$

and, using (3.18) and keeping in mind that $\tau \leqslant T$, we obtain

$$\left\| \frac{\partial c_\tau}{\partial x} \right\|^2_{L^2(0,T;H)} \leqslant \frac{\tau}{2} \|c_0\|^2_V + \frac{1}{2}(M_0 + c_b) + \frac{1}{2}(M_0 + c_b) \leqslant \frac{T}{2} \|c_0\|^2_V + M_0 + c_b.$$

In order to prove that c_τ is bounded in $H^1(0, T; H)$, it is enough to show that $\frac{\partial c_\tau}{\partial t}$ is bounded in $L^2(0, T; H)$ since the boundedness of c_τ in $L^2(0, T; H)$ has already been proven. Taking $v = c_s - c_{s-1} \in V$ as a test function in (3.14), we get, for a.e. $t \in (0, T)$ and $s = 1, \ldots, K$,

$$\int_0^l \frac{\partial c_\tau}{\partial t}(c_s - c_{s-1})\, dx + \frac{dF_\tau}{dt} \gamma_0(c_s - c_{s-1}) + \int_0^l \frac{\partial c_s}{\partial x} \frac{\partial (c_s - c_{s-1})}{\partial x} dx = 0.$$

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Then, considering (3.12) and (3.13), it follows that, for a.e. $t \in (0, T)$ and $s = 1, \ldots, K$,

$$\int_0^l \frac{(c_s - c_{s-1})^2}{\tau} dx + \frac{F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b)}{\tau} \gamma_0(c_s - c_{s-1}) + \int_0^l \frac{\partial c_s}{\partial x} \frac{\partial (c_s - c_{s-1})}{\partial x} dx = 0.$$

Using the fact that $x(x-y) \geqslant \frac{x^2}{2} - \frac{y^2}{2}$, for $x, y \in \mathbb{R}$, in the third term of the previous equality, we have, for $s = 1, \ldots, K$,

$$\int_0^l \frac{(c_s - c_{s-1})^2}{\tau} dx + \frac{F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b)}{\tau} \gamma_0(c_s - c_{s-1}) + \int_0^l \frac{1}{2} \left(\frac{\partial c_s}{\partial x} \right)^2 dx \leqslant \int_0^l \frac{1}{2} \left(\frac{\partial c_{s-1}}{\partial x} \right)^2 dx. \tag{3.32}$$

Now, using (3.2), we obtain, for $s = 1, \ldots, K$,

$$\int_0^l \frac{(c_s - c_{s-1})^2}{\tau} dx + \frac{(F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))^2}{\tau} + \int_0^l \frac{1}{2} \left(\frac{\partial c_s}{\partial x} \right)^2 dx \leqslant \int_0^l \frac{1}{2} \left(\frac{\partial c_{s-1}}{\partial x} \right)^2 dx.$$

Adding the term

$$\sum_{n=1}^{s-1} \left(\int_0^l \frac{(c_n - c_{n-1})^2}{\tau} dx + \frac{(F(\gamma_0(c_n) + c_b) - F(\gamma_0(c_{n-1}) + c_b))^2}{\tau} \right)$$

to both sides of the previous inequality, we find that, for $s = 1, \ldots, K$,

$$\sum_{n=1}^{s} \int_0^l \frac{(c_n - c_{n-1})^2}{\tau} dx + \sum_{n=1}^{s} \frac{\left(F(\gamma_0(c_n) + c_b) - F(\gamma_0(c_{n-1}) + c_b)\right)^2}{\tau} + \int_0^l \frac{1}{2} \left(\frac{\partial c_s}{\partial x} \right)^2 dx \leqslant \int_0^l \frac{1}{2} \left(\frac{\partial c_0}{\partial x} \right)^2 dx.$$

Then, since all terms of the left-hand side are nonnegative, it follows that, for $s = 1, \ldots, K$,

$$\sum_{n=1}^{s} \int_0^l \frac{(c_n - c_{n-1})^2}{\tau} dx \leqslant \int_0^l \frac{1}{2} \left(\frac{\partial c_0}{\partial x} \right)^2 dx, \tag{3.33}$$

$$\sum_{n=1}^{s} \frac{(F(\gamma_0(c_n) + c_b) - F(\gamma_0(c_{n-1}) + c_b))^2}{\tau} \leqslant \int_0^l \frac{1}{2} \left(\frac{\partial c_0}{\partial x} \right)^2 dx. \tag{3.34}$$

Therefore, using (3.12) and (3.33) we have

$$\left\|\frac{\partial c_\tau}{\partial t}\right\|^2_{L^2(0,T;H)} = \int_0^T \left\|\frac{\partial c_\tau}{\partial t}(t)\right\|^2_H dt = \sum_{s=1}^{K}\int_{(s-1)\tau}^{s\tau}\int_0^l \left(\frac{\partial c_\tau}{\partial t}(t,x)\right)^2 dx\,dt$$
$$= \sum_{s=1}^{K}\int_{(s-1)\tau}^{s\tau}\int_0^l \frac{(c_s-c_{s-1})^2}{\tau^2}dx\,dt = \sum_{s=1}^{K}\tau\int_0^l \frac{(c_s-c_{s-1})^2}{\tau^2}dx$$
$$\leqslant \int_0^l \frac{1}{2}\left(\frac{\partial c_0}{\partial x}\right)^2 dx = \frac{\|c_0\|_V^2}{2},$$

and the result follows.

Moreover, regarding F_τ and keeping in mind (3.13), we obtain

$$\|F_\tau\|^2_{H^1(0,T)} = \int_0^T |F_\tau(t)|^2 dt + \int_0^T \left|\frac{dF_\tau}{dt}(t)\right|^2 dt$$
$$\leqslant \sum_{s=1}^{K}\int_{(s-1)\tau}^{s\tau}\left(\left(s-\frac{t}{\tau}\right)|F(\gamma_0(c_{s-1})+c_b)|^2 + \left(\frac{t}{\tau}-s+1\right)|F(\gamma_0(c_s)+c_b)|^2\right)dt$$
$$+\sum_{s=1}^{K}\int_{(s-1)\tau}^{s\tau}\frac{(F(\gamma_0(c_s)+c_b)-F(\gamma_0(c_{s-1})+c_b))^2}{\tau^2}dt.$$

Taking into account that $|F(z)|\leqslant 1$, for all $z\in\mathbb{R}$, and applying (3.34), we get

$$\|F_\tau\|^2_{H^1(0,T)} \leqslant \sum_{s=1}^{K}\tau + \sum_{s=1}^{K}\tau\frac{(F(\gamma_0(c_s)+c_b)-F(\gamma_0(c_{s-1})+c_b))^2}{\tau^2}$$
$$\leqslant T + \int_0^l \frac{1}{2}\left(\frac{\partial c_0}{\partial x}\right)^2 dx = T + \frac{\|c_0\|_V^2}{2}.$$

Note also that

$$\|c_\tau-\tilde{c}_\tau\|^2_{L^2(0,T;H)} = \int_0^T \|c_\tau(t)-\tilde{c}_\tau(t)\|_H^2 dt$$
$$= \sum_{s=1}^{K}\int_{(s-1)\tau}^{s\tau}\left(\frac{t}{\tau}-s\right)^2\int_0^l (c_s(x)-c_{s-1}(x))^2 dx\,dt$$
$$= \sum_{s=1}^{K}\frac{\tau}{3}\int_0^l (c_s(x)-c_{s-1}(x))^2 dx$$
$$= \frac{\tau^2}{3}\sum_{s=1}^{K}\int_0^l \frac{(c_s(x)-c_{s-1}(x))^2}{\tau}dx,$$

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and using (3.33) we get

$$\|c_\tau - \tilde{c}_\tau\|^2_{L^2(0,T;H)} \leqslant \frac{\tau^2}{3}\int_0^l \frac{1}{2}\left(\frac{\partial c_0}{\partial x}\right)^2 dx = C_1\,\tau^2,$$

where $C_1 = \|c_0\|^2_V/6$. Finally, we find that

$$\begin{aligned}\|\gamma_0(c_\tau(t)) - \gamma_0(\tilde{c}_\tau(t))\|^2_{L^2(0,T)} &= \int_0^T |\gamma_0(c_\tau(t)) - \gamma_0(\tilde{c}_\tau(t))|^2 dt \\ &= \sum_{s=1}^{K}\int_{(s-1)\tau}^{s\tau}\left(\frac{t}{\tau} - s\right)^2 (\gamma_0(c_s) - \gamma_0(c_{s-1}))^2 dt \\ &= \frac{\tau^2}{3}\sum_{s=1}^{K}\frac{(\gamma_0(c_s) - \gamma_0(c_{s-1}))^2}{\tau}. \qquad (3.35)\end{aligned}$$

By using hypothesis (H1) for $\mathfrak{C} = c_b$ and Lemma 2, it follows that $-c_b \leqslant c_s \leqslant 0$ for $s = 1,\ldots,K$. Hence, we have

$$-c_b \leqslant \gamma_0(c_s) \leqslant 0, \qquad s = 1,\ldots,K, \qquad (3.36)$$

and then

$$0 \leqslant \gamma_0(c_s) + c_b \leqslant c_b, \qquad s = 1,\ldots,K. \qquad (3.37)$$

Considering the definition of function F and (3.36), we have, for $s = 1,\ldots,K$,

$$\begin{aligned}&(F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))(\gamma_0(c_s) - \gamma_0(c_{s-1})) \\ &\quad = \left(\frac{\gamma_0(c_s) + c_b}{1 + \gamma_0(c_s) + c_b} - \frac{\gamma_0(c_{s-1}) + c_b}{1 + \gamma_0(c_{s-1}) + c_b}\right)(\gamma_0(c_s) - \gamma_0(c_{s-1})) \\ &\quad = \frac{(\gamma_0(c_s) - \gamma_0(c_{s-1}))^2}{(1 + \gamma_0(c_s) + c_b)(1 + \gamma_0(c_{s-1}) + c_b)} \\ &\quad \geqslant \frac{(\gamma_0(c_s) - \gamma_0(c_{s-1}))^2}{(1 + c_b)^2},\end{aligned}$$

and, using this inequality in (3.32), we obtain, for $s = 1,\ldots,K$,

$$\int_0^l \frac{(c_s - c_{s-1})^2}{\tau}dx + \frac{(\gamma_0(c_s) - \gamma_0(c_{s-1}))^2}{\tau(1 + c_b)^2} + \int_0^l \frac{1}{2}\left(\frac{\partial c_s}{\partial x}\right)^2 dx \leqslant \int_0^l \frac{1}{2}\left(\frac{\partial c_{s-1}}{\partial x}\right)^2 dx.$$

Adding the term

$$\sum_{n=1}^{s-1}\left(\int_0^l \frac{(c_n - c_{n-1})^2}{\tau}dx + \frac{(\gamma_0(c_n) - \gamma_0(c_{n-1}))^2}{\tau(1 + c_b)^2}\right)$$

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to both sides of the previous inequality, we get, for $s = 1, \dots, K$,

$$\sum_{n=1}^{s} \int_0^l \frac{(c_n - c_{n-1})^2}{\tau} dx + \sum_{n=1}^{s} \frac{(\gamma_0(c_n) - \gamma_0(c_{n-1}))^2}{\tau(1+c_b)^2} + \int_0^l \frac{1}{2} \left(\frac{\partial c_s}{\partial x} \right)^2 dx$$
$$\leqslant \int_0^l \frac{1}{2} \left(\frac{\partial c_0}{\partial x} \right)^2 dx.$$

From this inequality, we have, for $s = 1, \dots, K$,

$$\sum_{n=1}^{s} \frac{(\gamma_0(c_n) - \gamma_0(c_{n-1}))^2}{\tau} \leqslant \frac{(1+c_b)^2}{2} \int_0^l \left(\frac{\partial c_0}{\partial x} \right)^2 dx,$$

and using this expression in (3.35), we conclude that

$$\|\gamma_0(c_\tau) - \gamma_0(\tilde{c})\|^2_{L^2(0,T)} \leqslant C_2 \tau^2,$$

where $C_2 = \frac{(1+c_b)^2}{6} \|c_0\|^2_V$. □

The following theorem establishes the existence of a unique solution to Problem P_W.

Theorem 3.3 *Assuming that hypothesis (H1) holds with $\mathfrak{C} = c_b$, then there exists a unique solution to Problem P_W with the regularity*

$$c \in H^1(0,T;H) \cap L^2(0,T;H^1(0,l)),$$
$$F(\gamma_0(c) + c_b) \in H^1(0,T), \quad F(\gamma_0(c(0)) + c_b) = F(\gamma_0(c_0) + c_b).$$

Moreover, this solution also satisfies

$$-c_b \leqslant c(t,x) \leqslant 0 \quad \text{a.e. in } Q_T = (0,T) \times (0,l). \tag{3.38}$$

Proof *Existence*. The estimates of Proposition 1 and the reflexivity of the space $L^2(0,T;V)$ lead to the existence of a function $c \in L^2(0,T;V)$ such that, for a subsequence (not relabelled),

$$\tilde{c}_\tau \rightharpoonup c \text{ weakly in } L^2(0,T;V), \tag{3.39}$$
$$c_\tau \rightharpoonup c \text{ weakly in } L^2(0,T;V). \tag{3.40}$$

Notice that the weak limits of these sequences coincide in $L^2(0,T;H)$ due to (3.27). Moreover, the estimates of Proposition 1 establish that the sequence c_τ is bounded in

$$W = \{u \in L^2(0,T;V); \quad \frac{\partial u}{\partial t} \in L^2(0,T;H)\}.$$

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Since W is reflexive, there exists an element $c_\star \in W$ and a subsequence, still denoted by τ, such that

$$c_\tau \rightharpoonup c_\star \text{ weakly in } W.$$

That is, we have

$$c_\tau \rightharpoonup c_\star \text{ weakly in } L^2(0,T;V), \quad \frac{\partial c_\tau}{\partial t} \rightharpoonup \frac{\partial c_\star}{\partial t} \text{ weakly in } L^2(0,T;H). \tag{3.41}$$

By the convergence (3.40) and the uniqueness of the weak limit we deduce that $c = c_\star$. Furthermore, using the Lions-Aubin Lemma (see [19]) with $B_0 = V$ and $B = B_1 = H$ and taking into account that the embedding $V \hookrightarrow H$ is compact, we get

$$c_\tau \to c \text{ in } L^2(0,T;H). \tag{3.42}$$

Moreover, since $H \hookrightarrow (H^1(0,l))'$, there exists a subsequence of c_τ (still relabelled by τ) weakly convergent to c in

$$W_1 = \{u \in L^2(0,T;H^1(0,l));\ \frac{\partial u}{\partial t} \in L^2(0,T;(H^1(0,l))')\}.$$

Taking into account the following space (see [17]):

$$W^{\varepsilon,2}(0,l) = \left\{ u \in H;\ \frac{|u(x)-u(y)|}{|x-y|^{\varepsilon+\frac{1}{2}}} \in L^2((0,l)\times(0,l)) \right\},$$

for $\frac{1}{2} < \varepsilon < 1$ and using the Lions-Aubin Lemma again, with $B_0 = H^1(0,l)$, $B = W^{\varepsilon,2}(0,l)$ and $B_1 = (H^1(0,l))'$ and regarding that $H^1(0,l) \hookrightarrow W^{\varepsilon,2}(0,l)$ is compact (see [17]) and $W^{\varepsilon,2}(0,l) \hookrightarrow (H^1(0,l))'$, we have

$$c_\tau \to c \text{ in } L^2(0,T;W^{\varepsilon,2}(0,l)).$$

Now, taking into account that the trace operator is linear and continuous (see [4]), we obtain

$$\gamma_0(c_\tau) \to \gamma_0(c) \text{ in } L^2(0,T).$$

Besides, using (3.28) we find that

$$\gamma_0(\tilde{c}_\tau) \to \gamma_0(c) \text{ in } L^2(0,T). \tag{3.43}$$

Since F_τ is bounded in $H^1(0,T)$ and this space is reflexive, we can extract a subsequence of τ, still denoted by τ, such that, for some $F_\star \in H^1(0,T)$, we get

$$F_\tau \rightharpoonup F_\star \text{ weakly in } H^1(0,T). \tag{3.44}$$

Due to the fact that the inclusion $H^1(0,T) \hookrightarrow L^2(0,T)$ is compact, it follows that

$$F_\tau \to F_\star \text{ in } L^2(0,T). \tag{3.45}$$

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Moreover, taking $t \in ((s-1)\tau, s\tau)$, $s = 1, \ldots, K$, and using

$$\begin{aligned}
&F_\tau(t) - F(\gamma_0(\tilde{c}_\tau(t)) + c_b) \\
&\quad = \left(s - \frac{t}{\tau}\right) F(\gamma_0(c_{s-1}) + c_b) + \left(\frac{t}{\tau} - s + 1\right) F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_s) + c_b) \\
&\quad = \left(\frac{t}{\tau} - s\right) (F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b)),
\end{aligned}$$

together with (3.34), we get

$$\begin{aligned}
\|F_\tau - F(\gamma_0(\tilde{c}_\tau) + c_b)\|^2_{L^2(0,T)} &= \int_0^T |F_\tau(t) - F(\gamma_0(\tilde{c}_\tau(t)) + c_b)|^2 dt \\
&= \sum_{s=1}^K \int_{(s-1)\tau}^{s\tau} \left(\frac{t}{\tau} - s\right)^2 (F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))^2 dt \\
&= \sum_{s=1}^K \frac{\tau}{3} (F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))^2 \\
&= \frac{\tau^2}{3} \sum_{s=1}^K \frac{(F(\gamma_0(c_s) + c_b) - F(\gamma_0(c_{s-1}) + c_b))^2}{\tau} \leqslant \tau^2 \frac{\|c_0\|_V^2}{6}.
\end{aligned}$$

Then, letting $\tau \to 0$, we deduce

$$F_\tau - F(\gamma_0(\tilde{c}_\tau) + c_b) \to 0 \quad \text{in} \quad L^2(0, T),$$

and using (3.43) and (3.45), we find that $F_\star = F(\gamma_0(c) + c_b)$ a.e. in $(0, T)$ and, consequently,

$$F_\tau \to F(\gamma_0(c) + c_b) \quad \text{in} \quad L^2(0, T). \tag{3.46}$$

Taking $v \in \mathscr{V}$, and integrating (3.14) from $t = 0$ to $t = T$, we obtain

$$\int_0^T \int_0^l \frac{\partial c_\tau}{\partial t} v \, dx \, dt + \int_0^T \frac{dF_\tau}{dt} \gamma_0(v) \, dt + \int_0^T \int_0^l \frac{\partial \tilde{c}_\tau}{\partial x} \frac{\partial v}{\partial x} dx \, dt = 0.$$

Using (3.39), (3.41) and (3.44) and passing to the limit when $\tau \to 0$,

$$\int_0^T \int_0^l \frac{\partial c}{\partial t} v \, dx \, dt + \int_0^T \frac{dF(\gamma_0(c) + c_b)}{dt} \gamma_0(v) \, dt + \int_0^T \int_0^l \frac{\partial c}{\partial x} \frac{\partial v}{\partial x} dx \, dt = 0$$

for any $v \in \mathscr{V}$, and therefore (2.17) holds. Moreover, let us take $v \in \mathscr{V}$ independent of t, that is to say $v(t, x) = v(x)$, using integration by parts and considering the definition of c_τ given in (3.10), we get, for a.e. $t \in (0, T)$,

$$\int_0^t \left(\frac{\partial c_\tau}{\partial t}(t), v\right)_H dt = (c_\tau(t), v)_H - (c_\tau(0), v)_H = (c_\tau(t), v)_H - (c_0, v)_H. \tag{3.47}$$

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Furthermore, using (3.42) we have

$$c_\tau(t) \longrightarrow c(t) \quad \text{in } H, \quad \text{for a.e. } t \in (0,T).$$

Thus, passing to the limit in (3.47), taking into account (3.41) and integration by parts, we obtain

$$(c(t),v)_H - (c(0),v)_H = \int_0^t \left(\frac{\partial c}{\partial t}(t), v\right)_H dt = (c(t),v)_H - (c_0,v)_H,$$

for a.e. $t \in (0,T)$. Therefore

$$(c(0) - c_0, v)_H = 0, \qquad \forall v \in V,$$

and, since V is dense in H, (2.18) holds a.e. in $(0,l)$.

Note also that, using integration by parts, we have

$$\int_0^t \frac{dF_\tau}{dt}(t)\,dt = F_\tau(t) - F_\tau(0) = F_\tau(t) - F(\gamma_0(c_0) + c_b), \quad \text{for a.e. } t \in (0,T).$$

Besides, using (3.46), passing to the limit in the previous expression and applying integration by parts, we get, for a.e. $t \in (0,T)$,

$$\begin{aligned} F(\gamma_0(c(t)) + c_b) - F(\gamma_0(c(0)) + c_b) &= \int_0^t \frac{dF(\gamma_0(c(t)) + c_b)}{dt}\,dt \\ &= F(\gamma_0(c(t)) + c_b) - F(\gamma_0(c_0) + c_b). \end{aligned}$$

Thus, the previous expression yields

$$F(\gamma_0(c(0)) + c_b) = F(\gamma_0(c_0) + c_b). \tag{3.48}$$

Using (3.27) and (3.42), we deduce that

$$\tilde{c}_\tau \to c \quad \text{in} \quad L^2(Q_T).$$

Then, for a subsequence (see [1])

$$\tilde{c}_\tau \to c \quad \text{a.e. in} \quad Q_T. \tag{3.49}$$

By using hypothesis (H1) with $\mathfrak{C} = c_b$, $-c_b \leqslant c_s(x) \leqslant 0$ a.e. in $(0,l)$ and then, by construction, $-c_b \leqslant \tilde{c}_\tau \leqslant 0$ also holds a.e. in Q_T. Thus, keeping in mind (3.49), we get (3.38).

Uniqueness. In order to prove the uniqueness of solution to Problem P_W, we proceed using several arguments already introduced in [11] which are detailed here for the reader's convenience. We consider $\psi \in V$ and we define

$$v_{\tau,n}(t,x) = \varphi_{\tau,n}(t)\psi(x),$$

where

$$\varphi_{\tau,n}(t) = \begin{cases} 1 & \text{if } t \in [0,\tau], \\ n(\tau - t) + 1 & \text{if } t \in [\tau, \tau + \frac{1}{n}], \\ 0 & \text{if } t \in [\tau + \frac{1}{n}, T], \end{cases}$$

for $\tau \in (0,T)$ and $n \in \mathbb{N}$. Since $v_{\tau,n} \in \mathscr{V}$, we can use it as a test function in equation (2.17) to get

$$\int_0^T \left\langle \frac{\partial c}{\partial t}(t), v_{\tau,n}(t) \right\rangle_{V' \times V} dt + \int_0^T ((c(t), v_{\tau,n}(t)))\, dt$$
$$+ \int_0^T \frac{d(F(\gamma_0(c(t)) + c_b))}{dt} \gamma_0(v_{\tau,n}(t))\, dt = 0. \tag{3.50}$$

Notice that $v_{\tau,n} \in H^1(0,T;V)$ and therefore, using Theorem 11.5 in [3] and taking into account that $v_{\tau,n}(T,x) = 0$ for a.e. $x \in (0,l)$, the first term of the previous expression reads, for all $\tau \in (0,T)$,

$$\int_0^T \left\langle \frac{\partial c}{\partial t}(t), v_{\tau,n}(t) \right\rangle_{V' \times V} dt = - \int_0^T \langle c(t), \frac{\partial v_{\tau,n}}{\partial t}(t) \rangle_{V \times V'} - (c(0), v_{\tau,n}(0))_H$$
$$= n \int_\tau^{\tau + \frac{1}{n}} (c(t), \psi)_H\, dt - (c_0, \psi)_H. \tag{3.51}$$

Furthermore, using integration by parts, considering $\varphi_{\tau,n}(T) = 0$ in the third term of equation (3.50) and taking into account expression (3.48), we obtain, for all $\tau \in (0,T)$,

$$\int_0^T \frac{d(F(\gamma_0(c(t)) + c_b))}{dt} \gamma_0(v_{\tau,n}(t))\, dt = - \int_0^T F(\gamma_0(c(t)) + c_b)\, \gamma_0(\psi)\, \frac{d\, \varphi_{\tau,n}}{dt}(t)\, dt$$
$$- F(\gamma_0(c_0) + c_b)\, \gamma_0(\psi)\, \varphi_{\tau,n}(0)$$
$$= \int_\tau^{\tau + \frac{1}{n}} n\, F(\gamma_0(c(t)) + c_b)\, \gamma_0(\psi)\, dt - F(\gamma_0(c_0) + c_b)\, \gamma_0(\psi). \tag{3.52}$$

Therefore, taking into account (3.51) and (3.52), equation (3.50) reads

$$\int_\tau^{\tau + \frac{1}{n}} (c(t), \psi)_H\, n\, dt + \int_0^T \varphi_{\tau,n}(t)\, ((c(t), \psi))\, dt + \int_\tau^{\tau + \frac{1}{n}} n\, F(\gamma_0(c(t)) + c_b)\, \gamma_0(\psi)\, dt$$
$$= (c_0, \psi)_H + F(\gamma_0(c_0) + c_b)\, \gamma_0(\psi), \qquad \forall \tau \in (0,T). \tag{3.53}$$

Now, let c_1 and c_2 be two solutions to Problem P_W. Subtracting the resulting equations obtained from the previous expression for $c = c_1$ and $c = c_2$, we get, for all $\tau \in (0,T)$,

$$\int_\tau^{\tau + \frac{1}{n}} (c_1(t) - c_2(t), \psi)_H\, n\, dt + \int_0^{\tau + \frac{1}{n}} ((c_1(t) - c_2(t), \psi)) \varphi_{\tau,n}(t)\, dt$$
$$+ \int_\tau^{\tau + \frac{1}{n}} (F(\gamma_0(c_1(t)) + c_b) - F(\gamma_0(c_2(t)) + c_b))\, n\, \gamma_0(\psi) = 0, \quad \forall \psi \in V. \tag{3.54}$$

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Taking into account that $c_1, c_2 \in \mathscr{W}(0,T) \subset \mathscr{C}([0,T];H)$ (see [18]) and using the mean value theorem, we have, for $t^\star \in [\tau, \tau+\frac{1}{n}]$,

$$\int_\tau^{\tau+\frac{1}{n}} (c_1(t)-c_2(t),\psi)_H\, n\, dt = (c_1(t^\star)-c_2(t^\star),\psi)_H. \tag{3.55}$$

We notice that

$$\int_0^{\tau+\frac{1}{n}} ((c_1(t)-c_2(t),\psi))\,\varphi_{\tau,n}(t)\,dt$$
$$= \int_0^T \chi\left(0,\tau+\frac{1}{n}\right) ((c_1(t)-c_2(t),\psi))\,\varphi_{\tau,n}(t)\,dt, \tag{3.56}$$

where $\chi(0,\tau+\frac{1}{n})$ denotes the characteristic function over the interval $(0,\tau+\frac{1}{n})$. Now, we define a sequence of functions given by

$$f_n(t) := \chi\left(0,\tau+\frac{1}{n}\right) ((c_1(t)-c_2(t),\psi))\varphi_{\tau,n}(t), \quad n \in \mathbb{N}.$$

We remark that $f_n \in L^1(0,T)$ for each $n \in \mathbb{N}$, and the family of functions f_n, $n \in \mathbb{N}$, satisfies

$$f_n(t) \longrightarrow f(t), \text{ a.e. } t \in (0,T),$$

where

$$f(t) = \chi(0,\tau)((c_1(t)-c_2(t),\psi))$$

and

$$|f_n(t)| \leqslant g(t), \text{ a.e. } t \in (0,T), \tag{3.57}$$

with

$$g(t) = ((c_1(t)-c_2(t),\psi)).$$

Then, applying the Lebesgue dominated convergence theorem, we can conclude that $f \in L^1(0,T)$ and

$$\int_0^{\tau+\frac{1}{n}} ((c_1(t)-c_2(t),\psi))\,\varphi_{\tau,n}(t)\,dt \longrightarrow \int_0^\tau ((c_1(t)-c_2(t),\psi))\,dt. \tag{3.58}$$

Moreover, considering that $F(\gamma_0(c_i(t))+c_b) \in H^1(0,T) \subset \mathscr{C}([0,T])$, for $i=1,2$, and using the mean value theorem, it follows that, for a given $t^{\star\star} \in [\tau,\tau+\frac{1}{n}]$,

$$\int_\tau^{\tau+\frac{1}{n}} (F(\gamma_0(c_1(t))+c_b) - F(\gamma_0(c_2(t))+c_b))\, n\, \psi(0)\,dt$$
$$= (F(\gamma_0(c_1(t^{\star\star}))+c_b) - F(\gamma_0(c_2(t^{\star\star}))+c_b))\,\psi(0). \tag{3.59}$$

Therefore, passing to the limit when $n \to \infty$ in (3.54) and taking into account (3.55),

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(3.58) and (3.59), it follows that, for all $\psi \in V$ and for a.e. $\tau \in (0, T)$,

$$(c_1(\tau) - c_2(\tau), \psi)_H + \int_0^\tau ((c_1(t) - c_2(t), \psi))\, dt$$
$$+(F(\gamma_0(c_1(\tau)) + c_b) - F(\gamma_0(c_2(\tau)) + c_b))\, \psi(0) = 0. \tag{3.60}$$

Now, we fix $\tau \in (0, T)$ and we take $\psi = c_1(\tau) - c_2(\tau)$ in (3.60) to obtain

$$\int_0^l (c_1(\tau, x) - c_2(\tau, x))^2 dx + \int_0^\tau ((c_1(t) - c_2(t), c_1(\tau) - c_2(\tau)))\, dt$$
$$+(F(\gamma_0(c_1(\tau)) + c_b) - F(\gamma_0(c_2(\tau)) + c_b))(\gamma_0(c_1(\tau)) - \gamma_0(c_2(\tau))) = 0.$$

Since F is nondecreasing, the last term of the previous equality is nonnegative, and then, for a.e. $\tau \in (0, T)$,

$$\|c_1(\tau) - c_2(\tau)\|_H^2$$
$$+ \int_0^\tau \int_0^l \left(\frac{\partial c_1}{\partial x}(t, x) - \frac{\partial c_2}{\partial x}(t, x) \right) \left(\frac{\partial c_1}{\partial x}(\tau, x) - \frac{\partial c_2}{\partial x}(\tau, x) \right) dx\, dt \leqslant 0. \tag{3.61}$$

Taking into account $\dfrac{\partial c_1}{\partial x} - \dfrac{\partial c_2}{\partial x} \in L^2(0, T; H)$, we define the function

$$\beta(\tau) := \int_0^\tau \left(\frac{\partial c_1}{\partial x}(s) - \frac{\partial c_2}{\partial x}(s) \right) ds$$

which belongs to $W^{1,2}(0, T; H)$ (see [19], page 104), and satisfies

$$\frac{d\beta}{d\tau}(\tau) = \frac{\partial c_1}{\partial x}(\tau) - \frac{\partial c_2}{\partial x}(\tau).$$

Thus, we deduce (see Chapter III, Corollary 1.1, in [19]),

$$\frac{1}{2} \frac{d}{d\tau} \|\beta(\tau)\|_H^2 = \left(\frac{d\beta}{d\tau}(\tau), \beta(\tau) \right)_H$$
$$= \int_0^l \int_0^\tau \left(\frac{\partial c_1}{\partial x}(s) - \frac{\partial c_2}{\partial x}(s) \right) ds \left(\frac{\partial c_1}{\partial x}(\tau) - \frac{\partial c_2}{\partial x}(\tau) \right) d\tau.$$

Therefore, taking into account the Fubini Theorem (see Theorem IV.5 in [1]), we can change the order of the integrals and then replace the previous equality in estimate (3.61) to obtain, for a.e. $\tau \in (0, T)$,

$$\|c_1(\tau) - c_2(\tau)\|_H^2 + \frac{1}{2} \frac{d}{d\tau} \|\beta(\tau)\|_H^2 \leqslant 0.$$

Integrating from 0 to T, we have

$$\int_0^T \|c_1(\tau) - c_2(\tau)\|_H^2 d\tau + \frac{1}{2} \int_0^T \frac{d}{d\tau} \|\beta(\tau)\|_H^2 d\tau \leqslant 0,$$

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and therefore

$$\int_0^T \|c_1(\tau) - c_2(\tau)\|_H^2 d\tau + \frac{1}{2}\|\beta(T)\|_H^2 \leqslant 0.$$

Consequently, $c_1 = c_2$ a.e in Q_T. □

4 Conclusions

A model was used to describe the dynamics of several surfactants at the air-water interface taking into account the Langmuir isotherm to tackle the time-dependent surface concentration. It introduced a nonlinearity at the boundary terms involving the time derivative of the solution. Existence of a bounded weak solution was obtained by using the Rothe method for a semi-discrete problem in time, and an uniqueness result was also stated.

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