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A nonlinear parabolic equation modelling surfactant diffusion

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An initial-boundary value problem for nonlinear parabolic equations modelling surfactant diffusions is investigated. The boundary conditions are of nonlinear adsorptive types, and the initial value has a single point jump. We study the well-posedness of the problem, the convergence of a numerical scheme, and the regularity as well as quantitative behaviour of solutions.

1 Introduction

In this paper, we are concerned with the well-posedness, regularity and quantitative properties of the solution for the following parabolic equation in spaces of one dimension with prescribed initial and boundary conditions (see Fig. 1):

$$(P) \quad \begin{cases} [A(u)]_t = u_{xx}, & x \in (0,1),\ t > 0, \\ u_x(1,t) = 0, & t > 0, \\ u_x(0,t) = [B(u(0,t))]_t, & t > 0, \\ u(x,0) = u_0(x), & x \in (0,1], \\ \lim_{t\to 0^+} B(u(0,t)) = B(\alpha), & x = 0, \end{cases} \tag{1.1}$$

where $A(\cdot)$ and $B(\cdot)$ are Lipschitz continuous functions satisfying, for some positive constants a and b,

$$A(0) = B(0) = 0, \quad a \leqslant A'(u) \leqslant b,\ 0 \leqslant B'(u) \leqslant b \quad \forall u \in R^1. \tag{1.2}$$

Problem (P) models the diffusion of a surfactant in a solution used in a photographic film coating process; see § 2 for a more detailed description of the model.

Mathematically, the unique features of (P) lie in the initial and boundary conditions. Notice that when $B(\alpha) \neq B(u_0(0))$, the initial conditions in problem (P) are different from the usual initial condition

$$u(x,0) = u_0(x), \quad 0 \leqslant x \leqslant 1.$$

Apparently, if $B(\alpha) \neq B(u_0(0))$ any solution $u(x,t)$ is not continuous at the corner $x = 0, t = 0$. It raises questions on the well-posedness and regularity of the solution.

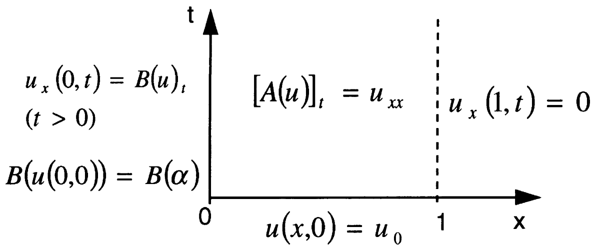

FIGURE 1. Illustration of problem (P).

On the other hand, one sees that in the range where $B' = 0$, the boundary condition is of the Neumann type. When $B' > 0$, however, it behaves like a Dirichlet boundary condition. In many physical situations, for instance the film coating problem presented here, $B'(u(0,t))$ may change from positive to zero at some time, or *vice versa*. Since it is not known *a priori* when $B' = 0$ and when $B' > 0$, this type of boundary condition provides a mathematical challenge. Clearly, a method that could automatically handle this sort of boundary condition may provide desirable numerical schemes.

Another motivation for our analysis of problem (P) originates from the numerical results in Barrick *et al.* [1]. In the numerical simulations, to take into account the singular initial condition, it is natural to take the initial value $u(x,0)$ as $u_0(x)$ for all $x \in (0,1]$ and α (in general, $u_0(0) \neq \alpha$) for $x = 0$; namely, take $u(x,0)$ as u_0 at all the grid points except for the origin, where the value of $u(0,0)$ is taken to be α. One would ask what the significance would be by simply changing the initial value at a single node, when the mesh size goes to zero. A direct observation shows that when $u_0(x)$ is a constant, $u \equiv u_0$ is an equilibrium state. Hence, we want to know whether the resulting approximate solutions tend to this trivial solution as the mesh size gets smaller and smaller. In addition, in certain ranges of physical parameters, we find that the numerical solutions tend to be unstable (i.e. sensitive to changes of parameters and mesh sizes). It seems important to address the following question: Is the instability due to mesh sizes, the singular behaviour of the initial data, or something else?

It is worth mentioning that for semi-linear parabolic equations, the boundary conditions of the type $\partial u/\partial n + au_t = G(x,t,u)$, where n is the exterior normal and a is non-negative, has been studied earlier by Ficken [2] and Friedman [3]. Uniqueness of the solution in the class of continuous function space was proved by Ficken [2] for the one-dimensional case, and by Friedman [3] for higher dimensional cases with more general space-time domains. However, because of the single point jump at $x = 0, t = 0$, a solution for problem (P) will neither be continuous nor in the Sobolev spaces. New treatments are needed for uniqueness.

The main purpose of the present paper is to carry out a rigorous mathematical study to problem (P). We will approach the problem based on a semi-discrete finite difference scheme. One advantage of such a constructive method is that we are able to use the scheme to perform the numerical simulations.

The rest of the paper is organized as follows. In § 2, we shall describe briefly the mathematical modelling. In § 3, we shall first define weak solutions for the problem (P), and then establish the uniqueness of weak solutions. In § 4, we prove the existence of weak solutions. In § 5, we study various properties of weak solutions, including regularity,

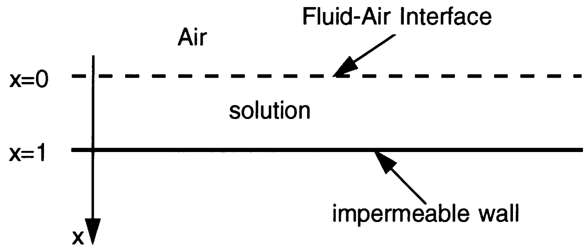

FIGURE 2. Schematic illustration of physical model.

long time behaviour and comparison principles. We shall also investigate the behaviour of the solution at the singular corner $x = 0, t = 0$. Some remarks regarding numerical simulations will be made in § 6.

2 Model description

In a film coating process, the fluid to be coated on the film is extruded from a slot in a container. Underneath the container lies the film backing which is moving horizontally. The fluid falls freely from the container to form a curtain-like flow, and eventually rests on the film to form a thin coating layer.

To increase the stability of the flow, a certain surfactant is added to the coating fluid. Surfactant is hydrophobic. When exposed to the air, the surfactant molecules move towards the fluid–air interface and accumulate there to form a thin layer like a 'skin' on the curtain like fluid. Due to certain special properties of surfactants (see Christian & Scameborn [4] for a detailed study), this thin layer of surfactant molecules decreases the surface tension of the fluid. Hence, by adjusting the concentration of the surfactant in the fluid, one is able to maintain the surface tension at an optimal level to avoid possible curling or dripping, and yet to keep the quality of the film and the cost. For more detailed description about the curtain coating, we refer to Friedman [5, chapter 6].

We now derive a mathematical model. By Frumpkin's law, the fluid surface tension γ (dyn/cm^2) is related to the surface concentration Γ (mol/cm^2) of surfactant via $\gamma = \gamma_0 + RK\Gamma_{\max} \ln(1 - \Gamma/\Gamma_{\max})$, where γ_0 is the surface tension of the fluid without surfactant, R the Boltzmann gas constant, K the Kelvin temperature, and $\Gamma_{\max}$ the maximum possible surface concentration of the surfactant. To calculate the surface concentration Γ of surfactant on the fluid–air interface, we assume the Langmuir isotherm equation [11]

$$\frac{\Gamma}{\Gamma_{\max}} = 1 - \frac{1}{1 + \beta C_{\text{top}}}, \tag{2.1}$$

where β (cm^3/mol) is the material constant and C_{top} (mol/cm^3) is the surfactant concentration in the fluid right underneath the fluid–air interface. Therefore, to compute the surface tension γ of the solution, we need to model the diffusion of the surfactants in the solution, and then compute the concentration C_{top} on the interface.

We assume that the curtain-like stream is flat, and that the fluid velocity is constant in every horizontal cross-section. The varying surface tension may drive a (Marangoni) flow due to the non-constant tangential stress at the interface. We assume that this flow is negligible compared to the base flow. We also assume that the surfactant diffusion in the vertical direction can be neglected. Then the distribution of surfactant on the horizontal cross-section at height h is the same as that obtained from a pure diffusion process in a 2D domain of the size of the cross-section of the curtain at time t, the amount of time needed for the cross-section to drop to the height h from the bottom of the coating fluid container. As pointed out by the referee, the condition for neglecting convection is that the diffusion timescale $L^2/D = O(1)$ while the Peclet number UL/D is much smaller. Hence, we can ignore the fluid motion, and simply consider only the pure diffusion of surfactant in a fixed 2D cross-section. Since the thickness of the curtain is much smaller than its width and length, we assume that the cross-section is an infinite slab, and that the surfactant concentration depends only upon the distance to the interface. The problem then reduces to the simple configuration that the surfactant solution is in an infinite slab with only one side open to the air (see Fig. 2). The other side of the slab is assumed to be a solid impermeable wall. In this configuration, we choose the coordinate system such that x is the distance to the interface. The interface is then $x = 0$, and the solid wall is located at $x = 1$.

Let $C(x,t)$ (mol/cm^3) be the bulk concentration of the surfactant in the fluid. When C becomes large, a certain amount of monomers (individual surfactant molecules) starts bounding together stably to form a micelle ('cluster'). Typically, a micelle consists of 60–200 monomers. This phenomenon slows down the diffusion process, since the micelles diffuse in the solution significantly slower than the monomers do, and they do not prefer to stay on the fluid–air interface. Therefore, the micelles make a negligible contribution to surface concentration, although the micelle diffusion inside the fluid is not negligible. Denote by C_{mon} and C_{mic} the monomer concentration and micelle concentration (mol/cm^3) respectively. Obviously, $C = C_{\text{mon}} + C_{\text{mic}}$. For the time scale of diffusion, which is also the magnitude of the time scale that a fluid particle reaches the film backing from the gate, it is reasonable to assume that there is a critical micellization concentration C_{cmc} such that when $C \leqslant C_{\text{cmc}}$, all the surfactant molecules in the solution always stay separately, i.e. $C = C_{\text{mon}}$. Otherwise, when $C > C_{\text{cmc}}$, the monomer concentration remains at its maximum level C_{cmc}, i.e. $C_{\text{mon}} = C_{\text{cmc}}$. We summarize these relations by

$$C_{\text{mon}} = \min\{C, C_{\text{cmc}}\}, \quad C_{\text{mic}} = \max\{C - C_{\text{cmc}}, 0\}, \quad C = C_{\text{mon}} + C_{\text{mic}}.$$

Denote by D_{mon} and D_{mic} ($D_{\text{mon}} > D_{\text{mic}}$) the diffusion coefficients of the monomers and micelles, respectively. By Fick's law, the concentration $C(x,t)$ satisfies

$$C_t = [D_{\text{mon}}(C_{\text{mon}})_x + D_{\text{mic}}(C_{\text{mic}})_x]_x.$$

Using the relation between $C_{\text{mon}}, C_{\text{mic}}$ and C, we may write it in the form

$$C_t = (D(C)C_x)_x, \qquad x \in (0,1),\ t > 0, \tag{2.2}$$

where $D(C)$ is defined by

$$D(C) = \begin{cases} D_{\text{mon}} & \text{if} \quad C \leqslant C_{\text{cmc}}, \\ D_{\text{mic}} & \text{if} \quad C > C_{\text{cmc}}. \end{cases}$$

At $x = 1$, we apply the no-flux condition

$$C_x(1,t) = 0 \qquad \text{for} \quad t > 0. \tag{2.3}$$

At the interface $x = 0$, conservation of mass leads to

$$(D(C)C_x)_{x=0} = \frac{\mathrm{d}}{\mathrm{d}t}\Gamma(t), \tag{2.4}$$

where $\Gamma(t)$ is the surface concentration at time t. Due to the time scale of the diffusion process, we may assume that the surface concentration instantaneously reaches equilibrium in response to the concentration C_{top}, i.e. the Langmuir isotherm equation (2.1) is valid. Hence $\Gamma(t)$ can be computed from C_{top} through (2.1). Since the accumulation of the micelles on the interface is negligible, we have $C_{top} = C_{\mathrm{mon}}(0,t) = \min\{C(0,t), C_{\mathrm{cmc}}\}$. By (2.1), condition (2.4) becomes

$$D(C(0,t))C_x(0,t) = \frac{\mathrm{d}}{\mathrm{d}t}\frac{-\Gamma_{\max}}{(1 + \beta\min\{C(0,t), C_{\mathrm{cmc}}\})}. \tag{2.5}$$

To impose an appropriate initial condition, we observe that initially (when the horizontal cross section of the curtain flow just exits from the container), the interface $x = 0$ is not exposed to air so that there is no surfactant molecule on the surface, i.e. $\Gamma(0) = 0$. Consequently, by (2.1), $C(0,0) = 0$. Therefore, to reflect this physical consideration, we impose the following initial condition:

$$C(\cdot,0) = C_0(\cdot), \qquad \lim_{t\searrow 0} C(0,t) = 0, \tag{2.6}$$

where $C_0(x)$, defined for $x \in (0,1]$, is the initial concentration of the surfactant solution, which typically is a constant function.

We thus derive the complete system (2.2), (2.3), (2.5) and (2.6) for the surfactant concentration C. For a more complete and more complicated model that takes into account various time scales and various sizes of micelles, see Friedman [5, chapter 6] and Swailes & Mckee [6], and the references therein.

To analyse the system, we introduce the new dependent variable u by

$$u = \begin{cases} D_{\mathrm{mon}}(C - C_{\mathrm{cmc}}) & \text{for } C \leqslant C_{\mathrm{cmc}}, \\ D_{\mathrm{mic}}(C - C_{\mathrm{cmc}}) & \text{for } C > C_{\mathrm{cmc}}. \end{cases}$$

Then, in the dimensionless form, the system (2.2), (2.3), (2.5), (2.6) becomes problem (P) with $A(u)$ and $B(u)$ being defined by

$$\begin{aligned} A(u) &= \begin{cases} u/D_{\mathrm{mon}} & \text{for } u \leqslant 0, \\ u/D_{\mathrm{mic}} & \text{for } u > 0, \end{cases} \\ B(u) &= \begin{cases} -\dfrac{\Gamma_{\max}}{1 + \beta(C_{\mathrm{cmc}} + u/D_{\mathrm{mon}})} + \dfrac{\Gamma_{\max}}{1 + \beta C_{\mathrm{cmc}}} & \text{for } u \leqslant 0, \\ 0 & \text{for } u > 0. \end{cases} \end{aligned} \tag{2.7}$$

Problem (P) was derived in particular for the film coating process. However, some analogous problems also appear in modelling many diffusion phenomenons in various industrial applications (see Cohen [7], for instance). Hence, in the rest of the paper, we shall consider, instead of the specific functions in (2.7), general Lipschitz continuous functions A and B satisfying (1.2). We point out that, since physically $C \geqslant 0$ (therefore $u \geqslant -D_{\mathrm{mon}}C_{\mathrm{cmc}}$), the function B defined in (2.7) can be modified to be a Lipschitz function in R^1, without changing the nature of the problem. In that sense, the assumptions in (1.2) hold for the model problem (2.2), (2.3), (2.5), (2.6).

3 Preliminary analysis

Throughout the paper, we shall always assume that the functions A and B are Lipschitz continuous in R and satisfy (1.2), and that $\alpha \in R^1$ and $u_0(\cdot) \in L^2((0,1))$.

We first introduce some notations. Let X be any Banach space and I be an open, or half-open half-closed, or closed interval in R^1. We denote by $L^2_{loc}(I;X)$ the space of all functions from I to X that are square integrable on any compact subset of I. The spaces $L^2(I;X), H^1(I;X)$, and $C^\gamma(I;X)$ $(0 \leqslant \gamma < 1)$ are defined in a similar manner.

We begin with the definition of a weak solution of (1.1).

Definition 3.1 A function $u(\cdot,t) \in L^2_{loc}([0,\infty);H^1((0,1)))$ is called a weak solution of problem (P) with initial data $(\alpha, u_0(\cdot))$ if for every $T > 0$ and every function $v \in C^1([0,1]\times[0,T])$ with $v(\cdot,T) = 0$, the following equation holds:

$$\int_0^T\int_0^1 [-A(u)v_t + u_x v_x]\mathrm{d}x\mathrm{d}t - \int_0^T B(u(0,t))v_t(0,t)\mathrm{d}t = \int_0^1 A(u_0(x))v(x,0)dx + B(\alpha)v(0,0). \qquad (3.1)$$

Remark 3.2 (1) Notice that $u \in L^2_{loc}([0,\infty);H^1((0,1)))$ implies that the mapping $x \in (0,1) \to u(x,\cdot)$ is in $H^1((0,1);L^2((0,T))) \subset C^{1/2}([0,1];L^2((0,T)))$. Hence the function $u(0,t)$ is uniquely defined and is in $L^2_{loc}([0,\infty))$. Consequently, since $B(\cdot)$ grows at most linearly, $B(u(0,\cdot))$ is well-defined and is in $L^2_{loc}([0,\infty))$. Hence, our weak solution is well-defined.

(2) By approximation if necessary, one can show that if u is a weak solution, then (3.1) holds for any test functions v satisfying

$$v_x \in L^2((0,1)\times(0,T)), \quad v_t \in C([0,1];L^2(0,T)), \quad v(\cdot,T) = 0. \qquad (3.2)$$

Here the constraint $v_t \in C([0,1];L^2((0,T)))$ is used to guarantee that the trace of v_t on $\{0\}\times(0,T)$ is well–defined.

(3) Under certain regularity assumptions, one can easily derive that a solution of (1.1) satisfies (3.1) so that it is a weak solution of (P). Later on in §4, we shall show that a weak solution of (P) satisfies (1.1) in certain Sobolev spaces, so that our weak formulation is equivalent to (1.1).

We now establish uniqueness of weak solutions.

Theorem 3.3 *Problem* (*P*) *admits at most one weak solution.*

Proof Assume that u_1 and u_2 are two solutions. Set $w = u_1 - u_2$. Then

$$\int_0^T\int_0^1 [(A(u_2) - A(u_2+w))\,v_t + w_x v_x]\,\mathrm{d}x\mathrm{d}t = \int_0^T [B(u_2+w) - B(u_2)]\,v_t|_{x=0}\mathrm{d}t \qquad (3.3)$$

for any v satisfying (3.2). Consider the function defined by $v(x,t) := \int_t^T w(x,\tau)\mathrm{d}\tau$. Then $v_t = -w \in L^2((0,T);H^1(0,1)) = H^1((0,1);L^2((0,T))) \subset C^{1/2}([0,1];L^2((0,T)))$. It then follows that v satisfies (3.2). Therefore, taking this v in (3.3) we obtain

$$\int_0^T\int_0^1 (A(u_2+w)-A(u_2))\,w\mathrm{d}x\mathrm{d}t+\int_0^T\int_0^1(-v_t)_x v_x\mathrm{d}x\mathrm{d}t + \int_0^T (B(u_2+w)-B(u_2))\,w|_{x=0}\mathrm{d}t=0.$$

Since A and B are non-decreasing functions, the first and third integrals are non-negative. Also, the second integral can be written as

$$\int_0^T\int_0^1(-v_t)_x v_x\mathrm{d}x\mathrm{d}t=-\frac{1}{2}\int_0^1\int_0^T((v_x)^2)_t\mathrm{d}t\mathrm{d}x=\frac{1}{2}\int_0^1(v_x(x,0))^2\mathrm{d}x\geqslant 0,$$

since $v_x(x,T)=0$. We thus conclude that $w\equiv 0$ which implies that $u_1=u_2$. □

Remark 3.4 (1) Notice that the dependence of the solution u on α is through $B(\alpha)$. Hence, if u is a weak solution with respect to (α, u_0), then it is also a weak solution with respect to $(\hat{\alpha}, u_0)$ provided that $B(\alpha)=B(\hat{\alpha})$. Physically, this is easy to understand, since B represents the surface concentration of the surfactant. Initially, we only count the surface concentration instead of the volume concentration.

(2) Clearly, if α and $\hat{\alpha}$ are two constants such that $B(\alpha)\neq B(\hat{\alpha})$, then the solutions corresponding to (α,u_0) and $(\hat{\alpha},u_0)$ are different.

(3) Suppose we replace $B(\alpha)$ in the definition of weak solutions by β; namely, consider the modified weak formulation for Problem (P): Find $u\in L^2_{loc}([0,\infty);H^1((0,1)))\cap C([0,\infty);L^2(0,1))$ such that, for any given $T>0$ and smooth v with $v(\cdot,T)=0$,

$$\int_0^T\int_0^1[-A(u)v_t+u_xv_x]\mathrm{d}x\mathrm{d}t-\int_0^T B(u(0,t))v_t(0,t)\mathrm{d}t=\int_0^1 A(u_0(x))v(x,0)\mathrm{d}x+\beta v(0,0).$$

Clearly, if $\beta\in B^{-1}(R^1)$, then by writing $\beta=B(\alpha)$, we know that the modified problem is equivalent to the original problem (P). However, if $\beta\notin B^{-1}(R^1)$, then we can show that this modified problem admits no weak solution. Here, we omit the details.

4 Existence of a weak solution

In this section, we shall prove that problem (P) has a weak solution. The idea of the proof is as follows. First, we construct approximate solutions via a semi-discrete finite difference scheme. Then we estimate the norms of the approximate solutions in certain functional spaces. Finally, we show that, as the mesh size approaches zero, a subsequence of the approximate solutions converges to a weak solution of (P). The uniqueness of the weak solution guarantees that the whole sequence will converge.

4.1 The finite difference scheme

Let $n\geqslant 3$ be the number of the spatial partitions, $h=1/n$ be the mesh size and $x_j=jh$, $j=0,\dots,n$ be the grid points. Denote by $U_j(t)$ the value of an approximate solution u^n at the grid point x_j, i.e. $U_j(t)=u^n(x_j,t)$. For convenience, we introduce the following notation:

$$DU_{j+\frac{1}{2}}(t) := \frac{U_{j+1}(t) - U_j(t)}{h},$$

$$D^2U_j(t) := \frac{U_{j+1} - 2U_j + U_{j-1}}{h^2} \equiv \frac{DU_{j+\frac{1}{2}} - DU_{j-\frac{1}{2}}}{h},$$

for $j = 0, ..., n-1$. Consider the following semi-discrete finite difference scheme for the problem (P):

$$(P^n) \quad \begin{cases} \dot{U}_j(t) = \dfrac{D^2U_j(t)}{A_n'(U_j)}, & j = 1, \dots, n-1, \ t > 0, \\ U_n(t) = U_{n-1}(t), & t \geqslant 0, \\ \dot{U}_0(t) = \dfrac{DU_{\frac{1}{2}}}{B_n'(U_0)}, & t > 0, \\ U_j(0) = \dfrac{1}{h}\displaystyle\int_{x_{j-1}}^{x_j} u_0(x)\mathrm{d}x, & j = 1, \dots, n-1, \\ U_0(0) = \alpha, & \end{cases}$$

where A_n and B_n are approximations of A and B with the following properties:

$$\begin{cases} A_n(\cdot), \ B_n(\cdot) \in C^2(R^1), \ A_n(0) = B_n(0) = 0, \\ |A_n(u) - A(u)| \leqslant 2h|u|, \ |B_n(u) - B(u)| \leqslant 2h|u|, \quad \forall u \in R^1, \\ a/2 \leqslant A_n'(u) \leqslant 2b, \ h \leqslant B_n'(u) \leqslant 2b \quad \forall u \in R^1, \end{cases} \tag{4.1}$$

where a and b are as in (1.2). Clearly, such approximations A_n and B_n exist.

Lemma 4.1 *Assume that A_n and B_n satisfy (4.1). Then for every $u_0 \in L^2((0,1))$, problem (P^n) has a unique solution for all $t \in [0, \infty)$.*

Proof We can use the relation $U_n = U_{n-1}$ to eliminate U_n from (P^n) to obtain an initial value problem for a system of n ordinary differential equations with n unknown functions $U := (U_0, \dots, U_{n-1})$. Since $(A_n'(u))^{-1}$ and $(B_n'(u))^{-1}$ are bounded smooth functions of $u \in R^1$, the right-hand side of the differential equations for U_j $(j = 0, \dots, n-1)$ is Lipschitz continuous and grows at most linearly with respect to $U_0, \dots, U_{n-1}$. Hence, by a standard theory of ordinary differential equations [8], this system has a unique solution for all $t \in [0, \infty)$. □

4.2 *A priori* estimates

To investigate the convergence of the finite difference scheme, we need to establish some *a priori* estimates.

Lemma 4.2 *Assume the conditions in Lemma 4.1. Let $U = (U_0, \dots, U_n)$ be the unique solution of (P^n). Then the following statements hold:*

(i) *For any $j = 0, \dots, n$ and any $t \geqslant 0$,*

$$\min\{U_0(0), \dots, U_{n-1}(0)\} \leqslant U_j(t) \leqslant \max\{U_0(0), \dots, U_{n-1}(0)\}. \tag{4.2}$$

(ii) *Let $\hat{B}_n(u)$ and $\hat{A}_n(u)$ be defined by*

$$\hat{A}_n(u) := \int_0^u sA_n'(s)\mathrm{d}s, \qquad \hat{B}_n(u) := \int_0^u sB_n'(s)\mathrm{d}s.$$

Then for any $t > 0$,

$$\hat{B}_n(U_0(t))+\sum_{j=1}^{n-1} h\hat{A}_n(U_j(t))+\int_0^t \sum_{j=1}^{n} h|DU_{j-\frac{1}{2}}(\tau)|^2 d\tau = \hat{B}_n(\alpha)+\sum_{j=1}^{n-1} h\hat{A}_n(U_j(0)). \tag{4.3}$$

(iii) *For any $t > 0$,*

$$\int_0^t \left[2B_n'(U_0)\dot{U}_0^2 + \sum_{j=1}^{n-1} h\left(A_n'(U_j)\dot{U}_j^2 + \frac{1}{A_n'(U_j)}|D^2U_j|^2\right)\right]\mathrm{d}\tau$$
$$+\sum_{i=1}^{n} h|DU_{j-\frac{1}{2}}(t)|^2 = \sum_{j=1}^{n-1} h|DU_{j-\frac{1}{2}}(0)|^2. \tag{4.4}$$

(iv) *For any $t > 0$,*

$$\int_0^t \tau\left[2B_n'(U_0)\dot{U}_0^2 + \sum_{j=1}^{n-1} h\left(A_n'(U_j)\dot{U}_j^2 + \frac{1}{A_n'(U_j)}|D^2U_j|^2\right)\right]\mathrm{d}\tau$$
$$+ t\sum_{i=1}^{n} h|DU_{j-\frac{1}{2}}(t)|^2 + \hat{B}_n(U_0(t)) + \sum_{j=1}^{n-1} h\hat{A}_n(U_j(t))$$
$$= \hat{B}_n(\alpha) + \sum_{j=1}^{n-1} h\hat{A}_n(U_j(0)). \tag{4.5}$$

Proof (i) We shall prove (4.2) by a contradiction argument.

Set $M = \max\{U_0(0), \dots, U_{n-1}(0)\}$. Suppose that the second inequality in (4.2) is not true. Then there exist $\varepsilon > 0$ and $\tau > 0$ such that

(a) $U_j < M + \varepsilon(1 + t)$ for all $t \in [0, \tau)$ and $j = 0, \dots, n-1$, and

(b) $U_{j^*}(\tau) = M + \varepsilon(1 + \tau)$ for some $j^* \in \{0, \dots, n-1\}$.

We now show that this is impossible.

Indeed, if $j^* = 0$ then $\dot{U}_{j^*}(\tau) = (U_1(\tau) - U_0(\tau))(hB(U_0'(\tau)))^{-1} \leqslant 0$. If $j^* \in \{1, \dots, n-1\}$, then $\dot{U}_{j^*}(\tau) = [U_{j^*+1}(\tau) - 2U_{j^*}(\tau) + U_{j^*-1}(\tau)]/[A_n'(U_j)h^2] \leqslant 0$. We have just proved that $\dot{U}_{j^*}(\tau) \leqslant 0$. On the other hand, the fact that $U_{j^*}(t) - [M + \varepsilon(1 + t)]$ as a function in $[0, \tau]$ reaches a maximum at $t = \tau$ implies that $\dot{U}_{j^*}(\tau) \geqslant \varepsilon > 0$. We thus obtain a contradiction. Hence the second inequality in (4.2) must hold for all $t \in [0, \infty)$. In a similar manner, we can show that the first inequality in (4.2) holds for all $t \in [0, \infty)$. This proves the first assertion of the lemma.

(ii) From the differential equation for U_j we have

$$0 = \sum_{j=1}^{n-1} hU_j\left\{A_n'(U_j)\dot{U}_j - \frac{DU_{j+\frac{1}{2}} - DU_{j-\frac{1}{2}}}{h}\right\}$$
$$= \sum_{j=1}^{n-1} hU_jA_n'(U_j)\dot{U}_j + \sum_{j=1}^{n} h|DU_{j-\frac{1}{2}}|^2 + \frac{U_0[U_1 - U_0]}{h},$$

where in the second equation, we have used the identity $DU_{n-\frac{1}{2}} = 0$. Using the equation for U_0, i.e. $B_n'(U_0)\dot{U}_0 = [U_1 - U_0]/h$ and using the definitions of $\hat{A}_n$ and $\hat{B}_n$, we obtain the identity

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{B}_n(U_0(t)) + \sum_{j=1}^{n-1} h\,\hat{A}_n(U_j(t))\right) + \sum_{j=1}^{n} h|DU_{j-\frac{1}{2}}(t)|^2 = 0. \tag{4.6}$$

Integrating this identity over $(0,t)$ yields the second assertion of the Lemma.

(iii) and (iv). Writing the differential equation for U_j $(1 \leqslant j \leqslant n-1)$ as $\sqrt{A_n{}'(U_j)}\dot{U}_j - (\sqrt{A_n{}'(U_j)})^{-1}D^2U_j = 0$, we obtain

$$\begin{aligned}
0 &= \sum_{j=1}^{n-1} h\left(\sqrt{A_n'(U_j)}\dot{U}_j - \frac{1}{\sqrt{A_n'(U_j)}}D^2U_j\right)^2 \\
&= \sum_{j=1}^{n-1}\left(hA_n'(U_j)\dot{U}_j^2 + \frac{h}{A_n'(U_j)}|D^2U_j|^2 - 2\dot{U}_j\left(DU_{j+\frac{1}{2}} - DU_{j-\frac{1}{2}}\right)\right) \\
&= \sum_{j=1}^{n-1} h\left(A_n'(U_j)\dot{U}_j^2 + \frac{1}{A_n'(U_j)}|D^2U_j|^2 + 2DU_{j-\frac{1}{2}}\frac{\mathrm{d}}{\mathrm{d}t}DU_{j-\frac{1}{2}}\right) + 2\dot{U}_0DU_{\frac{1}{2}}.
\end{aligned}$$

Using the relations $DU_{n-\frac{1}{2}} = 0$ and $DU_{\frac{1}{2}} = B_n'(U_0)\dot{U}_0$, we then obtain

$$0 = \sum_{j=1}^{n-1} h\left(A_n'(U_j)\dot{U}_j^2 + \frac{1}{A_n'(U_j)}|D^2U_j|^2\right) + 2B_n'(U_0)\dot{U}_0^2 + \frac{\mathrm{d}}{\mathrm{d}t}\sum_{j=1}^{n} h|DU_{j-\frac{1}{2}}|^2.$$

Integrating this identity over $(0,t)$, we obtain (iii). This identity also implies that

$$\begin{aligned}
&t\sum_{j=1}^{n-1} h\left(A_n'(U_j)\dot{U}_j^2 + \frac{|D^2U_j|^2}{A_n'(U_j)}\right) + 2tB_n'(U_0)\dot{U}_0^2 + \frac{\mathrm{d}}{\mathrm{d}t}\left(t\sum_{j=1}^{n} h|DU_{j-\frac{1}{2}}|^2\right) \\
&\quad = \sum_{j=1}^{n} h|DU_{j-\frac{1}{2}}|^2 \\
&\quad = -\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{B}_n(U_0(t)) + \sum_{j=1}^{n-1} h\hat{A}_n(U_j(t))\right) \quad \text{(by (4.6))}.
\end{aligned}$$

Integrating the above relation over $(0,t)$, we obtain (4.5), thereby completing the proof of the lemma. □

4.3 Existence

With the help of Lemma 4.2, we are now ready to prove the existence of a weak solution to Problem (P). For convenience, we introduce functions $\hat{B}(u)$ and $\hat{A}(u)$ by

$$\hat{A}(u) := \int_0^u sA'(s)\mathrm{d}s, \qquad \hat{B}(u) := \int_0^u sB'(s)\mathrm{d}s.$$

Theorem 4.1 *Assume that A and B satisfy* (1.2). *Also assume that* $\alpha \in R, u_0 \in L^2((0,1))$.

Then problem (P) *admits a unique weak solution u. In addition, we have* $\sqrt{t}u_t, \sqrt{t}u_{xx} \in L^2((0,1)\times(0,\infty))$ *and for any* $T > 0$,

$$\hat{B}(u(0,T)) + \int_0^1 \hat{A}(u(x,T))\mathrm{d}x + \int_0^T\int_0^1 u_x^2\mathrm{d}x \leqslant \hat{B}(\alpha) + \int_0^1 \hat{A}(u_0(x))\mathrm{d}x, \tag{4.7}$$

$$\begin{aligned}\int_0^T \left(tB'(u(0,t))u_t^2(0,t) + \int_0^1 \left(tA'(u)u_t^2 + \frac{t}{A'(u)}u_{xx}^2\right)\mathrm{d}x\right)\mathrm{d}t \\ + \int_0^1 Tu_x^2(x,T)\mathrm{d}x + \int_0^1 \hat{A}(u(x,T))\mathrm{d}x + \hat{B}(u(0,T)) \\ \leqslant \int_0^1 \hat{A}(u_0(x))\mathrm{d}x + \hat{B}(\alpha).\end{aligned} \tag{4.8}$$

Furthermore, if $u_0 \in L^\infty((0,1))$, *then*

$$\|u\|_{L^\infty((0,1)\times(0,\infty))} \leqslant \max\{|\alpha|, \|u_0\|_{L^\infty((0,1))}\}. \tag{4.9}$$

If $u_0 \in H^1((0,1))$ *and* $u_0(0) = \alpha$ *then, for any* $T > 0$,

$$\begin{aligned}\int_0^T \left(B'(u(0,t))(u_t(0,t))^2 + \int_0^1 \left(A'(u)u_t^2 + \frac{1}{A'(u)}u_{xx}^2\right)\mathrm{d}x\right)\mathrm{d}t \\ + \int_0^1 u_x^2(x,t)\mathrm{d}x \leqslant \int_0^1 u_{0_x}^2(x)\mathrm{d}x.\end{aligned} \tag{4.10}$$

Proof For every fixed integer $n \geqslant 3$, let $U^n(t) = \{U_0(t),\ldots,U_{n-1}(t)\}$ be the solution to problem (P^n). We define a sequence of piecewise linear functions $\{u^n(x,t)\}$ by

$$u^n(x,t) = U_{j-1}(t) + (x-(j-1)h)DU_{j-\frac{1}{2}}(t),$$

$$\forall\, t \geqslant 0,\ x \in ((j-1)h, jh),\ j = 1,\ldots,n.$$

Clearly, u^n is Lipschitz continuous in $[0,1]\times[0,\infty)$, and

$$u_x^n(x,t) = DU_{j-\frac{1}{2}}(t), \quad \forall\, t \geqslant 0,\ x \in ((j-1)h, jh).$$

By (ii) of Lemma 4.2, we have

$$\int_0^\infty\int_0^1 (u_x^n)^2\mathrm{d}x\mathrm{d}t = \int_0^\infty \sum_{j=1}^n h|DU_{j-\frac{1}{2}}|^2\mathrm{d}t \leqslant \hat{B}_n(\alpha) + \sum_{j=1}^{n-1} h\hat{A}_n(U_j(0)). \tag{4.11}$$

By (4.1) and the definition of $U_j(0)$, $\sum_{j=1}^n h\hat{A}_n(U_j(0)) \leqslant C_1(1 + \int_0^1 u_0^2\mathrm{d}x)$ where C_1 is a constant independent of n. Hence, the right-hand side of (4.11) is uniformly (in n) bounded. That is,

$$\sup_{n\geqslant 3}\int_0^\infty\int_0^1 |u_x^n|^2\mathrm{d}x\mathrm{d}t < C_2, \tag{4.12}$$

where (and in the rest of the section) C_2 is a constant depending only on the initial data.

Similarly, since $\hat{A}_n(s) \geqslant a|s|^2$ for all $s \in R^1$, (4.3) implies that

$$\sup_{n \geqslant 3} \left(\sup_{t > 0} \int_0^1 (u^n(\cdot, t))^2 \mathrm{d}x \right) < C_2. \tag{4.13}$$

Finally,

$$\begin{aligned}
\int_0^1 |u_t^n(x,t)|^2 \mathrm{d}x &= \frac{h}{3} \sum_{j=1}^{n} (\dot{U}_{j-1}^2 + \dot{U}_j \dot{U}_{j-1} + \dot{U}_j^2) \leqslant \frac{h}{2} \sum_{j=1}^{n} (\dot{U}_{j-1}^2 + \dot{U}_j^2) \\
&= \frac{h}{2} (\dot{U}_0(t)^2 + \dot{U}_n^2) + \sum_{i=1}^{n-1} h \dot{U}_j^2 \\
&\leqslant \max\left(\frac{h}{\min B_n'}, \frac{1}{\min A_n'} \right) \left(B_n'(U_0) \dot{U}_0^2 + 2h \sum_{i=1}^{n} A_n'(U_j) \dot{U}_j^2 \right).
\end{aligned}$$

It then follows from (4.1) and (4.5) that

$$\sup_{n \geqslant 3} \int_0^\infty \int_0^1 t (u_t^n(x,t))^2 \mathrm{d}x \mathrm{d}t < C_2.$$

This estimate, together with (4.12) and (4.13), implies that there exist a function $u \in L^2_{\mathrm{loc}}([0,\infty); H^1((0,1)))$ and a subsequence $\{n_i\}_{i=1}^\infty$ such that, as $i \to \infty, n_i \to \infty$,

$$\begin{aligned}
&u^{n_i} \longrightarrow u && \text{in} \quad L^2_{\mathrm{loc}}([0,1] \times [0,\infty)), \\
&u^{n_i} \longrightarrow u && \text{weakly in} \quad L^2((0,T); H^1((0,T))), \\
&A_n(u^{n_i}) \longrightarrow A(u) && \text{in} \quad L^2_{\mathrm{loc}}([0,1] \times [0,\infty)), \\
&u^{n_i}(0,t) \longrightarrow u(0,t) && \text{in} \quad L^2_{\mathrm{loc}}([0,\infty)), \\
&B_n(u^{n_i}(0,t)) \longrightarrow B(u(0,t)) && \text{in} \quad L^2_{\mathrm{loc}}([0,\infty)), \\
&A_n(u^{n_i}(x,0)) \longrightarrow A(u_0(x)) && \text{in} \quad L^2((0,1)),
\end{aligned}$$

for any $T > 0$. Now we show that u is a weak solution of problem (P).

Let $T > 0$ be any given number and v be any given smooth function with $v(\cdot, T) \equiv 0$. Using the relations

$$D^2 U_j = [DU_{j+\frac{1}{2}} - DU_{j-\frac{1}{2}}]/h = [u_x^n(x+h,t) - u_x^n(x,t)]/h$$

for all $x \in (x_{j-1}, x_j)$ and $u_x^n(x,t) = DU_{n-\frac{1}{2}} = 0$ for all $x \in (1-h, 1)$, we obtain

$$\begin{aligned}
&\sum_{j=1}^{n-1} [A_n(U_j)]_t \int_{(j-1)h}^{jh} v(x,t) \mathrm{d}x = \sum_{j=1}^{n-1} D^2 U_j \int_{(j-1)h}^{jh} v(x,t) \mathrm{d}x \\
&= \sum_{j=1}^{n-1} \int_{(j-1)h}^{jh} \frac{u_x^n(x+h,t) - u_x^n(x)}{h} v(x,t) \mathrm{d}x \\
&= -\int_0^1 u_x^n \frac{v(x,t) - v(x-h,t)}{h} \mathrm{d}x - DU_{\frac{1}{2}} \frac{1}{h} \int_{-h}^0 v(x,t) \mathrm{d}x \\
&= -\int_0^1 u_x^n \frac{v(x,t) - v(x-h)}{h} \mathrm{d}x - [B_n(u^n(0,t))]_t \frac{1}{h} \int_{-h}^0 v(x,t) \mathrm{d}x.
\end{aligned}$$

It follows that

$$\int_0^T \sum_{j=1}^{n-1}[A_n(U_j)]_t \int_{(j-1)h}^{jh} v(x,t)\mathrm{d}x\mathrm{d}t$$
$$= -\int_0^T \int_0^1 u_x^n \frac{v(x,t)-v(x-h)}{h}\mathrm{d}x\mathrm{d}t + \int_0^T B_n(u^n(0,t))\frac{1}{h}\int_{-h}^0 v_t(x,t)\mathrm{d}x\mathrm{d}t$$
$$+B_n(\alpha)\frac{1}{h}\int_{-h}^0 v(x,0)\mathrm{d}x. \tag{4.14}$$

We point out that $B_n(\alpha)$ in the last term comes from the condition $U_0(0) = \alpha$. Define a step function $\tilde{u}^n(x,t)$ by

$$\tilde{u}^n(x,t) = U_j(t), \quad t \geqslant 0, \quad x \in [(j-1)h, jh), \quad j = 1,\ldots,n.$$

Then the left-hand side of (4.14) can also be written as

$$\int_0^T \sum_{j=1}^{n-1}[A_n(U_j)]_t \int_{(j-1)h}^{jh} v(x,t)\mathrm{d}x\mathrm{d}t$$
$$= \int_0^T \int_0^{1-h} A_n(\tilde{u}^n)_t v(x,t)\mathrm{d}x\mathrm{d}t$$
$$= -\int_0^T \int_0^{1-h} A_n(\tilde{u}^n)v_t\mathrm{d}x\mathrm{d}t - \int_0^{1-h} A_n(\tilde{u}^n(x,0))v(x,0)\mathrm{d}x.$$

Combining this with (4.14) we get

$$\int_0^T \int_0^1 \left(-A_n(\tilde{u}^n)v_t + u_x^n\frac{v(x,t)-v(x-h,t)}{h}\right)\mathrm{d}x\mathrm{d}t - \int_0^T B_n(u^n(0,t))\frac{1}{h}\int_{-h}^0 v_t(x,t)\mathrm{d}x\mathrm{d}t$$
$$= \int_0^{1-h} A_n(\tilde{u}^n(x,0))v(x,0)dx + B(\alpha)\frac{1}{h}\int_{-h}^0 v(x,0)\mathrm{d}x. \tag{4.15}$$

By Lemma 4.2, we find that

$$\int_0^T \int_0^1 |\tilde{u}^n - u^n|^2\mathrm{d}x\mathrm{d}t = \frac{h^2}{3}\int_0^T \sum_{j=1}^n h|DU_{j-\frac{1}{2}}|^2\mathrm{d}t \to 0$$

as $n \to \infty$, so that as $i \to \infty$, $\tilde{u}^{n_i} \to u$ in $L^2_{\mathrm{loc}}([0,1] \times [0,\infty))$. Thus, taking $n = n_i$ in (4.15) and sending i to ∞, we obtain

$$\int_0^T \int_0^1 [-A(u)v_t + u_x v_x]\mathrm{d}x\mathrm{d}t - \int_0^T B(u(0,t))v_t(0,t)\mathrm{d}t$$
$$= B(\alpha)v(0,0) + \int_0^1 A(u_0(x))v(x,0)\mathrm{d}x.$$

This shows that $u(x,t)$ is a weak solution of (P) for Uniqueness follows from Theorem 2.1.

The estimates (4.7)–(4.10) follow from the estimates in Lemma 4.2 and standard theory of finite difference approximations (for instance, see Ciarlet & Lions [9]). Here, we omit the details. □

5 Properties of weak solutions

5.1 Strong solutions

In this subsection, we show that any weak solution of (P) does satisfy (1.1) in a certain sense. First, we collect some of the estimates regarding the regularity of the weak solution obtained in the previous section.

Theorem 5.1 *Assume that $A(\cdot)$ and $B(\cdot)$ satisfy* (1.2), *and that $u_0(\cdot) \in L^2((0,1))$. Then the weak solution u for problem (P) satisfies*

$$u_x,\ \sqrt{t}u_t,\ \sqrt{t}u_{xx} \in L^2((0,1)\times(0,\infty)), \tag{5.1}$$

$$u,\ \sqrt{t}u_x \in L^\infty((0,\infty);L^2((0,1))), \tag{5.2}$$

$$u \in C^{1/2,1/4}([0,1]\times[\delta,T]) \qquad \forall\, 0<\delta<T<\infty. \tag{5.3}$$

Moreover, if $u_0(\cdot) \in H^1((0,1))$ and $\alpha = u_0(0)$, then $u_t,\ u_{xx} \in L^2((0,1)\times(0,\infty))$, $u_x \in L^\infty((0,\infty);L^2((0,1)))$, and $u \in C^{1/2,1/4}([0,1]\times[0,T])$ for any $T>0$.

Proof The assertions (5.1) and (5.2) follow from the estimates (4.7) and (4.8) we obtained in Theorem 4.1. The assertion (5.3) follows from a standard Sobolev embedding theorem [10]: $L^\infty((\delta,T);H^1((0,1))) \cap H^1((\delta,T);L^2((0,1))) \subset C^{1/2,1/4}([0,1]\times[\delta,T])$. The last assertion also follows from Theorem 4.1. □

Now we can show that any weak solution satisfies (1.1) in certain Sobolev spaces.

Theorem 5.2 *Assume that $u^0 \in L^2((0,1))$. Then the weak solution u of* (P) *is a strong solution of* (1.1) *in the following sense:*

(i) $u_t, u_{xx} \in L^2_{\text{loc}}([0,1]\times(0,\infty))$ *and* $[A(u)]_t = u_{xx}$ *a.e. in* $(0,1)\times(0,\infty)$;

(ii) $u(x,t) \in C([0,1]\times(0,\infty))$, *and* $u_x(1,t)=0$, $\quad (B(u(0,t)))_t = u_x(0,t) \in L^2_{\text{loc}}((0,\infty))$;

(iii) *For any* $p\in[1,2)$, $u \in C([0,\infty);L^p((0,1)))$ *and* $u(\cdot,0)=u_0(\cdot)$;

(iv) $\lim_{t\searrow 0} B(u(0,t)) = B(\alpha)$.

Proof (i) The first assertion follows from Theorem 5.1 and the fact that identity (3.1) implies that $[A(u)]_t - u_{xx} = 0$ in the distribution sense.

(ii) Using the first assertion and taking proper test functions in (3.1), we can derive that $\int_0^\infty u_x(1,t)z(t)\mathrm{d}t = 0$ and $\int_0^\infty [B(u(0,t))z_t(t) + u_x(0,t)z(t)]\mathrm{d}t = 0$ for any smooth function with compact support on $(0,\infty)$. It then follows that $u_x(1,t)=0$ in $L^2_{\text{loc}}((0,\infty))$ and $[B(u(0,t))]_t = u_x(0,t)$ in the distribution sense. Since $u_x(0,t) \in L^2_{\text{loc}}((0,\infty))$, we then also know that $[B(u(0,t))]_t = u_x(0,t)$ in $L^2_{\text{loc}}((0,\infty))$.

(iii) Since u is a weak solution of $[A(u)]_t = u_{xx}$ in $(0,1)\times(0,\infty)$ with initial data $u_0(x)$ and the boundary condition $u_x(1,t)=0$, by the theory of parabolic equations [10], for any $\delta>0$, $\lim_{t\searrow 0}\|u(\cdot,t)-u_0(\cdot)\|_{L^2((\delta,1))} = 0$. Also, since $u \in L^\infty((0,\infty);L^2((0,1)))$, we have, for any $p\in[1,2)$,

$$\|u(\cdot,t)-u_0(\cdot)\|_{L^p((0,\delta))} \leqslant \|u(\cdot,t)-u_0\|_{L^2((0,1))}\delta^{1-p/2} \leqslant C\delta^{1-p/2},$$

where C is independent of t. Hence, as $t \searrow 0$, $u(\cdot, t) \to u_0(\cdot)$ in $L^p((0,1))$.

(iv) We first claim that for every $t > 0$,

$$\int_0^1 A(u(x,t))\mathrm{d}x + B(u(0,t)) = \int_0^1 A(u_0(x))\mathrm{d}x + B(\alpha), \tag{5.4}$$

for all $t > 0$. In fact, let $\zeta(s)$ be a function defined by $\zeta(s) = 0$ for $s \geqslant 0$, $\zeta(s) = s$ for $s \in [-1, 0]$ and $\zeta = -1$ for $s \leqslant -1$. Taking $v(x, \tau) = \zeta(\frac{\tau - t}{\varepsilon})$ with $\varepsilon > 0$ in (3.1) and sending $\varepsilon \searrow 0$, we obtain the assertion (5.4).

We can now use (iii), the Lipschitz continuity of $A(\cdot)$, and (5.4) to conclude that

$$\lim_{t\searrow 0} |B(u(0,t)) - B(\alpha)| = \lim_{t\searrow 0} |\int_0^1 A(u(x,t)) - A(u_0(x))|\mathrm{d}x = 0.$$

This concludes the proof of the theorem. □

Remark 5.3 The identity (5.4) stands for the conservation of mass. In fact, $A(u(\cdot, t))$ is the concentration of the surfactant in the solution, and $B(u)$ is the amount of surfactant on the surface, so the left-hand side of (5.4) is the total amount of surfactant.

5.2 A comparison principle

Theorem 5.4 *Assume that α^1 and α^2 are two real numbers satisfying $B(\alpha^1) \leqslant B(\alpha^2)$ and that $u_0^1(\cdot)$ and $u_0^2(\cdot)$ are two $L^2((0,1))$ functions satisfying $u_0^1(x) \leqslant u_0^2(x)$ for a.e. x. Let u^1 and u^2 be two solutions of problem (P) with respect to (α^1, u_0^1) and (α^2, u_0^2). Then*

$$u^1(x,t) \leqslant u^2(x,t) \quad \forall\, x \in [0,1],\ t > 0.$$

Moreover, if for some $x^* \in [0,1]$, $t^* > 0$, $u^1(x^*, t^*) = u^2(x^*, t^*)$, then $B(\alpha^1) = B(\alpha^2)$ and $u_0^1(\cdot) \equiv u_0^2(\cdot)$.

Proof Since the weak solution depends on α only through $B(\alpha)$, we can assume without loss of generality that $\alpha_1 \leqslant \alpha_2$. For convenience, we also assume that $u_0^1(x) \leqslant u_0^2(x)$ for all x

For any fixed n, let $(U_0^i(t), \ldots, U_n^i(t))$ be the solution of the semi–discrete finite difference scheme (P^n) with $\alpha = \alpha^i$ and $u_0 = u_0^i$, $i = 1, 2$. Then use the same method that we used to prove the first assertion of Lemma 4.2, we can show that $U_j^1(\cdot) \leqslant U_j^2(\cdot)$ for all $j = 0, \ldots, n$. Hence, since the weak solution of (P) can be obtained as the limit of the solution of (P^n), we obtain that $u^1 \leqslant u^2$.

Now assume that for some $t^* > 0$, $x^* \in [0,1]$, $u^1(x^*, t^*) = u^2(x^*, t^*)$. If $x^* > 0$, then since $u^1 \leqslant u^2$ on the parabolic boundary of $[0,1] \times [0, t^*]$, we conclude from the strong comparison principle for parabolic equations that $u^1 \equiv u^2$ in $[0,1] \times [0, \tau^*]$. If $x^* = 0$, then $(0, t^*)$ is a minimum of $u^2 - u^1$ in $[0,1] \times [0, \tau^*]$. we claim that $u^1 \equiv u^2$. In fact, if $u^1 \not\equiv u^2$ in $(0,1) \times (0, t^*)$, then by the Hopf maximum principle, $(u_2 - u_1)_x(0, t^*) > 0$. On the other hand, we have

$$\begin{aligned}(u_2 - u_1)_x(0, t^*) &= \frac{\mathrm{d}}{\mathrm{d}t}(B(u^2(0, t^*)) - B(u^1(0, t^*))) \\ &= B'(u^2(0, t^*))\frac{\mathrm{d}}{\mathrm{d}t}(u^2(0, t^*) - u^1(0, t^*)) \leqslant 0,\end{aligned}$$

a contradiction. Hence, we must have $u^1 \equiv u^2$. It then follows from the weak formulation that $u_0^1 = u_0^2$ and $B(\alpha^1) = B(\alpha^2)$. This completes the proof of the theorem. $\square$

5.3 Behaviour of weak solutions near $(0,0)$

Let u be the solution to problem (P) with the initial data (α, u_0). Set $[\alpha_1, \alpha_2] = \{s \mid B(s) = \alpha\}$. By (iv) of Theorem 5.2 and the monotonicity of B, it is easy to see that

$$\alpha_1 \leqslant \liminf_{t \searrow 0} u(0,t) \leqslant \limsup_{t \searrow 0} u(0,t) \leqslant \alpha_2. \tag{5.5}$$

Theorem 5.5 *Assume (1.2) and $u_0 \in L^2((0,1))$, and that u is the solution to problem (P) with the initial data (α, u_0). Then the following holds:*

(i) *If $\alpha_1 = \alpha_2$, then $\lim_{t\searrow 0} u(0,t) = \alpha$.*

(ii) *If $\alpha_1 < \alpha_2$, then the following results hold:*

  (a) *If $\liminf_{x\searrow 0} u_0(x) \geqslant \alpha_2$, then $\lim_{t\searrow 0} u(0,t) = \alpha_2$;*

  (b) *If $\limsup_{x\searrow 0} u_0(x) \leqslant \alpha_1$, then $\lim_{t\searrow 0} u(0,t) = \alpha_1$;*

  (c) *If $\gamma = \lim_{x\searrow 0} u_0(x)$ exists and $\gamma \in [\alpha_1, \alpha_2]$, then $\lim_{t\searrow 0} u(0,t) = \gamma = \lim_{x\searrow 0} u_0(x)$.*

(iii) *The weak solution u is continuous at $(0,0)$ if and only if $u_0(0+) := \lim_{x\searrow 0} u_0(x)$ exists, and $B(\alpha) = B(u_0(0+))$.*

Proof (i) The first assertion follows immediately from (5.5).

(ii) (a) By (5.5), we need only to show that $\liminf_{t\searrow 0} u(0,t) \geqslant \alpha_2$.

Let $\beta \in (\alpha_1, \alpha_2)$ be any fixed constant. Let $\hat{u}_0(\cdot) \in L^2((0,1))$ be a function such that $\hat{u}_0 \leqslant u_0$ in $(0,1)$ and $u_0(x) = \beta$ in $[0,\delta]$ for some $\delta > 0$. Let $\hat{u}$ be the solution to the equation $[A(\hat{u})]_t = \hat{u}_{xx}$ subject to the initial conditions $\hat{u}(x,0) = \hat{u}_0(x)$ and homogeneous Neumann boundary condition $\hat{u}_x(0,t) = \hat{u}_x(1,t) = 0$. Then by the classical theory of parabolic equations [10], $\hat{u}$ is continuous near $(0,0)$ and therefore, $\hat{u} \in (\alpha_1, \alpha_2)$ in a neighborhood of $(0,0)$. Namely, $B(\hat{u}) = B(\alpha)$ in a neighborhood of origin, so that $[B(\hat{u}(0,t))]_t = 0 = u_x(0,t)$ provide that t is small enough. Therefore, it can be shown that $\hat{u}$ is a weak solution of (P) with respect to $(\beta, \hat{u}_0)$ in a small time interval. Consequently, by the comparison principle, we have $u(0,t) \geqslant \hat{u}(0,t)$ for all t sufficiently small. It then follows that $\liminf_{t\searrow 0} u(0,t) \geqslant \lim_{t\searrow 0} \hat{u}(0,t) = \beta$. Since β is an arbitrary number in (α_1, α_2), we then have $\liminf_{t\searrow 0} u(0,t) \geqslant \alpha_2$. Hence, $\lim_{t\searrow 0} u(0,t)$ exists and equals to α_2

(ii) (b) The proof follows the same argument as in part (a) and is omitted.

(ii) (c) Let $\hat{u}$ be the solution of (1.1) with the third and fifth conditions be replaced by the Neumann boundary condition. Then same argument as in (ii) (a) yields $u = \hat{u}$ for sufficiently small t. Since $\hat{u}$ is continuous near the origin, we then know that $\lim_{t\searrow 0} u(0,t) = \gamma$.

(iii) From the previous two assertions, we know that $\lim_{t\searrow 0} u(0,t) = u_0(0+)$. Now consider $\tilde{u}$ as the solution of (1.1) with the third and fifth condition be replaced by $\tilde{u}(0,t) = u(0,t)$. Since $u(0,0+) = u_0(0+)$, we know that $\tilde{u}$ is continuous at $(0,0)$ Obviously, $u = \tilde{u}$, so, we know that u is continuous at $(0,0)$. $\square$

5.4 Asymptotic behaviour as $t \to \infty$

Theorem 5.6 *Assume* (1.2) *and* $u_0 \in L^2((0,1))$. *Then as* $t \to \infty$,

$$u(\cdot, t) \longrightarrow \beta \quad \text{in} \quad C^{1/2}([0,1]),$$

where β *is the unique solution to the algebraic equation*

$$B(\beta) + A(\beta) = B(\alpha) + \int_0^1 A(u_0(x))\mathrm{d}x. \tag{5.6}$$

Physically the assertion of the theorem means that the surfactant diffusion process will reach an equilibrium as time goes to infinity.

Proof Since $\sqrt{t}u_x(\cdot, t) \in L^\infty((0,\infty); L^2(0,1))$,

$$\|u_x(\cdot, t)\|_{L^2((0,1))} \leqslant C/t \qquad \forall\, t > 0,$$

where C is a constant independent of t. Also $u(\cdot, t)$ is uniformly bounded in $L^2((0,1))$ (by (4.7) in Theorem 4.1). Hence, for any sequence $\{t_n\}$ with $\lim_{n\to\infty} t_n = \infty$, there is a subsequence $\{t_{n_j}\}$ with $\lim_{j\to\infty} n_j = \infty$ such that $u(\cdot, t_{n_j})$ approaches to a constant function in $C^\gamma([0,1])$ for any $\gamma \in (0, 1/2)$. Denote this constant by β. Then from the identity (5.4), β satisfies (5.6), so that it is unique. Therefore, the whole family $\{u(\cdot, t)\}_{t>0}$ approaches the constant function β as $t \to \infty$. The convergence is under the norm of $H^1((0,1))$, and consequently, also under the norm of $C^{1/2}([0,1])$. □

5.5 Stability with respect to the physical data

Theorem 5.7 *Let* $\{A^\varepsilon\}_{0<\varepsilon\leqslant 1}$ *and* $\{B^\varepsilon\}_{0<\varepsilon\leqslant 1}$ *be families of Lipschitz continuous functions such that for every* $\varepsilon \in (0,1]$, A^ε *and* B^ε *satisfy* (1.2). *Also let* $\{\alpha^\varepsilon\}_{0<\varepsilon\leqslant 1}$ *be a family of real numbers and* $\{u_0^\varepsilon(\cdot)\}_{0<\varepsilon\leqslant 1}$ *be a family of functions uniformly bounded in* $L^2((0,1))$. *Assume that as* $\varepsilon \searrow 0$,

$$A^\varepsilon(\cdot) \to A(\cdot), \quad B^\varepsilon(\cdot) \to B(\cdot)$$

uniformly in any compact set of R^1 *, and that*

$$u_0^\varepsilon(\cdot) \to u_0(\cdot) \ \text{ in } \quad L^2((0,1)), \quad \alpha^\varepsilon \to \alpha.$$

Let u *be the solution of problem (P) and* u^ε, $0 < \varepsilon \leqslant 1$, *be the solution of* (P) *with* A, B, u_0, α *being replaced by* $A^\varepsilon, B^\varepsilon, u_0^\varepsilon, \alpha^\varepsilon$ *respectively. Then, as* $\varepsilon \to 0$, $u^\varepsilon \to u$ *in* $C^{\gamma,\gamma/2}([0,1] \times [\delta, T])$ *for any* $\gamma \in (0, 1/2)$ *and any* $\delta > 0$ *and* $T > \delta$.

Proof By the *a priori* estimates in Theorem 4.1, for any $\delta \in (0,1)$, the family of the solutions $\{u^\varepsilon\}$ is uniform bounded in $H^1((0,1) \times (\delta, \frac{1}{\delta}))$ and in $L^\infty\left([0,T]; L^2((0,1))\right)$. Hence any subsequence of $\{u^\varepsilon\}$ has a subsequence that is convergent a.e. in $(0,1) \times (0,T)$, and weakly in $L^2((0,T); H^1((0,1)))$. In addition, the trace of the subsequence on $\{0\} \times (0,T)$ converges in $L^2((0,T))$. It then follows from the identities (3.1) that the limit is a weak solution of (P). Since weak solutions of (P) is unique, we then deduce that the whole sequence $\{u^\varepsilon\}$ converges to u a.e. in $(0,1) \times (0,T)$. From Theorem 4.1, the family $\{u^\varepsilon\}$ is a bounded sequence in $C^{1/2,1/4}([0,1] \times [\delta, T])$, we thus conclude that the convergence is also in $C^{\gamma,\gamma/2}([0,1] \times [\delta, T])$ for any $\gamma \in (0, 1/2)$. □

5.6 Monotonicity

In this subsection, we assume that $u_0 \in C^1([0,1])$ and

$$\alpha \leqslant u_0(0), \quad u_0'(x) \geqslant 0 \quad \forall\, x \in [0,1]. \tag{5.7}$$

In fact, the model problem in § 1 yields the condition $u_0(x) = D_1(c_0 - C_{\text{cmc}})$ and $\alpha = -D_1\, C_{\text{cmc}}$ where c_0 is a constant representing the initial volume surfactant concentration. Clearly, such initial data satisfies (5.7).

Theorem 5.8 *Assume* (5.7). *Then the solution u of* (P) *satisfies*

$$u_x(x,t) \geqslant 0 \quad \forall x \in (0,1), t > 0.$$

In addition, equality holds if and only if u_0 is a constant function and $B(\alpha) = B(u_0(0))$. Furthermore, $B(u(0,t))$ is a non-decreasing function of t.

Proof First, we consider the case that $\alpha < u_0(0)$ and $u_0' > 0$ in $[0,1]$. For any integer $n \geqslant 3$, consider the solution $(U_0, \ldots, U_n)$ to the problem (P^n). We claim that for all $t \geqslant 0$,

$$U_j(t) < U_{j+1}(t) \quad \forall\, j = 0, \ldots, n-2. \tag{5.8}$$

First of all, by the continuity of $U_j(\cdot)$ and the assumption that $\alpha < u_0(0)$ and $u_0' > 0$, (5.8) holds for all small t. Hence, if (5.8) does not hold for all $t \geqslant 0$, then there exists a first $T > 0$ such that (5.8) holds for all $t \in [0, T)$, and for some $j^* \in \{0, \ldots, n-2\}$, $U_{j^*}(T) = U_{j^*+1}(T)$. We claim this is impossible. We consider two situations: (i) $j \in \{1, \ldots, n-2\}$ and (ii) $j^* = 0$.

In the case (i), setting $e(t) = U_{j^*+1} - U_{j^*}$, we have, from the differential equation for U_j and U_{j+1}, that

$$\frac{\mathrm{d}}{\mathrm{d}t} e(t) + \frac{2}{h^2} e(t) = \frac{1}{h^2}[U_{j^*} - U_{j^*-1}] + \frac{1}{h^2}[U_{j^*+2} - U_{j^*+1}] > 0 \quad \forall t \in [0, T).$$

Since $e(0) > 0$, we know that $e(T) > 0$, which contradicts to the assumption that $e(T) = U_{j^*+1} - U_{j^*} = 0$.

In case (ii), we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(U_1 - U_0) &= \frac{1}{h^2}\left((U_2 - U_1) + \left[-1 - \frac{h}{B_n'(U_0)}\right](U_1 - U_0)\right) \\ &> \frac{1}{h^2}\left(-1 - \frac{h}{B_n'(U_0)}\right)(U_1 - U_0) \quad \forall\, t \in [0, T).\end{aligned}$$

Since $U_1(0) - U_0(0) > 0$, we then conclude that $U_1(T) - U_0(T) > 0$. Again, this contradicts the assumption that $U_{j^*}(T) = U_{j^*+1}(T)$.

Once we find that (5.8) holds for all $t \in [0, \infty)$, we can then deduce that u, the limit of the solution of (P^n) as $n \to \infty$, satisfies $u_x \geqslant 0$ in $(0,1) \times (0, \infty)$.

Now, suppose we only have $u_0' \geqslant 0$ and $B(\alpha) \leqslant B(u_0(0))$. We take an approximation sequence $(\alpha^\varepsilon, u_0^\varepsilon)$ which approaches (α, u_0) and satisfies $\alpha^\varepsilon < u_0^\varepsilon(0), u_{0x}^\varepsilon > 0$. Then by the previous analysis and the stability result of Theorem 5.7, we conclude that $u_x \geqslant 0$ in $(0, 1) \times (0, \infty)$. Noticing that $w = u_x$ satisfies the parabolic equation $(A'(u)w)_t = w_{xx}$ in $(0, 1) \times (0, \infty)$. By the strong maximum principle, the non-negativity of w then implies that either $w > 0$ in $(0, 1) \times (0, \infty)$ or $w \equiv 0$.

Finally, since $B(u(0, t))_t = u_x(0, t) \geqslant 0$, we then know that $B(u(0, t))$ is non-decreasing. □

Remark 5.9 The conclusion that $B(u(0, 1))$ is non-decreasing means that the surface concentration increases until it reaches its maximum.

6 Conclusion

The mathematical model (P) is well-posed, and the semi-discrete finite difference scheme (P^n) is convergent. We thus justify mathematically that the single point jump of initial value must be taken into account in designing numerical schemes.

In the model, we have assumed that the velocity of the fluid is the same in every horizontal cross-section, and there is no diffusion between the horizontal cross sections. A full model would include the transportation term. In such a case, one needs to couple problem (P) with a free boundary problem for the fluid–air interface, in which free boundary conditions would also depend on the surface tension. This would be a quite challenging problem.

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