



Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Numerical analysis of an adsorption dynamic model at the air–water interface[☆]

M.I.M. Copetti^a, J.R. Fernández^{b,*}, M.C. Muñoz^c, C. Núñez^c^a *Laboratório de Análise Numérica e Astrofísica, Departamento de Matemática, Universidade Federal de Santa Maria, 97105-900, Santa Maria, RS, Brazil*^b *Departamento de Matemática Aplicada I, Universidade de Vigo, ETSI Telecomunicación, Campus As Lagoas Marcosende s/n, 36310 Vigo, Spain*^c *Departamento de Didáctica de las Ciencias Experimentales, Facultad de Ciencias de la Educación, Campus Norte, 15782 Santiago de Compostela, Spain*

HIGHLIGHTS

- An adsorption dynamic model for surfactants is numerically studied.
- A priori error estimates are proved by using Gronwall's inequality.
- Linear convergence is obtained using regularity and an interpolation operator.
- Numerical results show the accuracy and the performance of the approximations.

ARTICLE INFO

Article history:

Received 30 May 2013

Received in revised form 3 September 2013

Keywords:

Adsorption dynamic model
Surfactant
Langmuir isotherm
Finite element approximation
Error estimates
Numerical simulations

ABSTRACT

In this paper we deal with the numerical analysis of an adsorption dynamic model arising in a surfactant solution at the air–water interface; the diffusion model is considered together with the so-called Langmuir isotherm. An existence and uniqueness result is stated. Then, fully discrete approximations are introduced by using a finite element method and a hybrid combination of backward and forward Euler schemes. Error estimates are proved from which, under adequate additional regularity conditions, the linear convergence of the algorithm is derived assuming a dependence between both spatial and time discretization parameters. Finally, some numerical simulations are presented in order to demonstrate the accuracy of the algorithm and the behaviour of the solution for two commercially available surfactants.

© 2014 Elsevier B.V. All rights reserved.

1. Introduction

The study of surfactant adsorption dynamics at the air–water interface has been shown as a determinant issue for its application in areas such as biochemistry, medicine, agrochemistry, metallurgy, food processing and so on (see, for instance, the review paper [1]). A newly formed surface in a surfactant solution is accomplished with the incorporation of surfactant

[☆] The work of J.R. Fernández, M.C. Muñoz and C. Núñez has been supported by Xunta de Galicia under the research project PGIDIT 10PXIB291088PR and the Ministerio de Economía y Competitividad under the research project MTM2012-36452-C02-02, and the work of M.I.M. Copetti has been partially supported by CNPq (grant 302425/2011-0) and CAPES (grant 8659-11-7).

* Correspondence to: Departamento de Matemática Aplicada I, Universidade de Vigo, ETSI de Telecomunicación, Buzón 104, Campus As Lagoas Marcosende s/n, 36310 Vigo, Spain.

E-mail addresses: mimcopetti@ufsm.br (M.I.M. Copetti), jose.fernandez@uvigo.es (J.R. Fernández), mcarmen.muniz@usc.es (M.C. Muñoz), crisrina.nunez.garcia@usc.es (C. Núñez).

<http://dx.doi.org/10.1016/j.cam.2014.11.063>

0377-0427/© 2014 Elsevier B.V. All rights reserved.

molecules to this surface, drastically reducing its surface tension. This dynamic process may vary depending on its temperature, salinity, type of surfactant and concentration, ranging from milliseconds to several hours in order to reach its equilibrium. The analysis of the dynamic surface tension is then closely related to the transportation of molecules as a consequence of both a diffusion and an adsorption–desorption mechanisms from the bulk of the solution to the interface and vice versa. As it is well-known, from the mathematical point of view, this process is modelled by using the classical partial differential equation of diffusion in one spatial dimension, coupled with the corresponding adsorption model by means of a suitable boundary condition at the subsurface, the unknowns being both bulk and surface concentrations. The paper by Ward and Tordai [2] was the first mathematical research concerned in achieving analytical solutions for the diffusion controlled model, considering infinite diffusion length and then obtaining approximations for long and short times. Even if numerical methods have been developed for the approximation of different nonlinear isotherms (see, e.g., [1,3,4]), to our knowledge the numerical analysis of some of these approximations is unknown yet. Therefore, in this paper we consider the classical and well-known Langmuir's isotherm, which leads to a nonlinear boundary condition between both surface and subsurface concentrations, for a finite diffusion length. This problem has been mathematically analysed in the recently published paper [5], where the existence of a unique weak solution was proved by using Rothe's method and fixed-point arguments. Thus, this paper is parallel to [5] and it continues the research started in [6], where the simplest (linear) Henry's isotherm was analysed.

The outline of this paper is as follows. In Section 2, we briefly describe the mathematical model and we introduce its variational formulation, for which an existence and uniqueness result, recently proved in [5], is stated. Then, fully discrete approximations are introduced in Section 3 by using a finite element method for the spatial approximation and a hybrid combination of backward and forward Euler schemes for the discretization of the time derivatives. An error estimate result is proved from which the linear convergence is deduced under suitable regularity assumptions and a dependence between the two discretization parameters. Finally, in Section 4 some numerical examples are shown to demonstrate the accuracy of the algorithm and the behaviour of the solution for two commercially available surfactants.

2. The model and its variational formulation

In order to introduce the whole dynamic process, it is important to take into account the boundary called *subsurface*, located a few molecular diameters below the air–water interface, and splitting the domain where only diffusion takes place and the region in which only adsorption–desorption occurs.

Let us denote by x the distance from the interface and $\tilde{c}(t, x)$ the concentration of surfactant at point $x \in [0, l]$ and time $t \in [0, T]$; l and T being the length of the recipient and the final time, respectively. The boundary $x = 0$ of the spatial interval corresponds to the location of the subsurface. Denoting by $\Gamma(t)$ the time-dependent surface concentration and taking into account Fick's law, we consider the diffusion partial differential equation:

$$\frac{\partial \tilde{c}}{\partial t}(t, x) - D \frac{\partial^2 \tilde{c}}{\partial x^2}(t, x) = 0, \quad x \in (0, l), \quad t > 0, \quad (1)$$

together with the boundary conditions (see [1,7]):

$$D \frac{\partial \tilde{c}}{\partial x}(t, 0) = \frac{d\Gamma}{dt}(t), \quad t > 0, \quad (2)$$

$$\tilde{c}(t, l) = c_b, \quad t > 0, \quad (3)$$

and the initial conditions:

$$\tilde{c}(0, x) = \tilde{c}_0(x), \quad x \in (0, l), \quad (4)$$

$$\Gamma(0) = \Gamma_0. \quad (5)$$

In Eqs. (1)–(3), $D > 0$ is the diffusion coefficient and the positive constant c_b is the bulk concentration. Besides, $\tilde{c}_0(x)$ is a function defined in $[0, l]$ and being equal to c_b on $x = l$. We remark that the time-dependent surface concentration, $\Gamma(t)$, actually becomes an unknown of the system and then an additional condition must be given in order to close the problem. Hereafter, we consider the well-known and classical Langmuir isotherm (see [1]):

$$\Gamma(t) = \Gamma_m \frac{K_L \tilde{c}(t, 0)}{1 + K_L \tilde{c}(t, 0)}, \quad (6)$$

where Γ_m is the maximum surface concentration and K_L is the Langmuir equilibrium adsorption constant. Here, the parameter Γ_m is a theoretical limit that cannot normally be reached because the surfactant solutions in this study are assumed to remain below the critical micelle concentration. Moreover, it is worth noticing that the surfactant concentration in (6) is assumed to be nonnegative and, as it is known, at low concentrations, or when $K_L \tilde{c}(t) \ll 1$, the Langmuir isotherm can be approximated by the Henry isotherm.

For the sake of clarity in the presentation we assume that the constants D , K_L and Γ_m are equal to 1.

Computing the derivative of the Langmuir isotherm (6), boundary condition (2) can be written in the form:

$$\frac{\partial \tilde{c}}{\partial x}(t, 0) = \frac{\frac{\partial \tilde{c}}{\partial t}(t, 0)}{(1 + \tilde{c}(t, 0))^2}, \quad t > 0. \quad (7)$$

Download English Version:

<https://daneshyari.com/en/article/6422464>

Download Persian Version:

<https://daneshyari.com/article/6422464>

[Daneshyari.com](https://daneshyari.com)