Study of a pseudo-stationary state for a corrosion model: Existence and numerical approximation

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A B S T R A C T

In this paper, we consider a system of partial differential equations describing the pseudo-stationary state of a dense oxide layer. We investigate the question of existence of a solution to the system and we design a numerical scheme for its approximation. Numerical experiments with real-life data shows the efficiency of the method. Then, the analysis is fulfilled on a simplified model.

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1. Introduction

1.1. General framework of the study

The concept for long term storage of high-level radioactive waste in France under study is based on an underground repository. The waste shall be confined in a glass matrix and then placed into cylindrical steel canisters. These containers shall be placed into micro-tunnels in the highly impermeable Callovo-Oxfordian claystone layer at a depth of several hundred metres.

The long-term safety assessment of the geological repository has to take into account the degradation of the carbon steel used for the waste overpacks and the cell disposal liners, which are in contact with the claystone formation. This degradation is mainly caused by generalized corrosion processes which take place under anaerobic conditions. As a tool to investigate the corrosion processes at the surface of the carbon

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steel canisters, the Diffusion Poisson Coupled Model (DPCM) for corrosion has been developed by Bataillon et al. [1].

The DPCM model describes the evolution of a dense oxide layer in the region of contact between the claystones and the metal. This is based on a coupled system of electromigration–diffusion equations for the transport of the charge carriers in the oxide layer, and a Poisson equation for the electric potential. The interactions between the oxide layer and the clay soil or the metal are described in terms of Robin boundary conditions. The system includes moving boundary equations based on the Pilling–Bedworth ratio [2]. As the oxide layer is very thin compared to the waste overpack size, the model proposed in [1] is a one-dimensional model.

The questions of existence of a solution to the full DPCM model and of long-time behaviour are still open questions, due to the complexity of the model. However, some results have been obtained for a simplified model where only two species of charge carriers (electrons and ferric cations) are taken into account and where the domain is fixed. In [3], Chainais-Hillairet and Lacroix-Violet prove the existence of an evolutive solution for this simplified model, while [4] deals with the existence of a stationary solution.

In [5], Bataillon et al. proposed a numerical method for the approximation of the DPCM model. This numerical scheme has been implemented in the simulation code CALIPSO, developed at ANDRA (the French nuclear waste management agency). The convergence of the scheme has been established by Chainais-Hillairet, Colin and Lacroix-Violet in [6] for the two-species model on a fixed domain. The long time simulations presented in [5] highlighted the existence of a pseudo stationary state: a state where all the density profiles, as the profile of the electric potential and the size of the oxide layer, are constant, while both interfaces are moving at the same velocity. Moreover, it appears that the pseudo stationary state can be reached more or less quickly depending on the value of the pH.

In many cases of application, the significant solution to the DPCM model may be the pseudo stationary one and in order to reduce the numerical costs, it is interesting to propose a scheme for its direct computation. Therefore, we propose in this paper an efficient numerical method for the approximation of the pseudo stationary state of the DPCM model. Moreover, we investigate the question of existence of a pseudo steady state on a simplified model. We also justify our choice of scheme with the study of its application to the simplified model: we will see that the scheme that we propose is exact in this case. The existence of a pseudo steady state is not so obvious and seems strongly related to the boundary conditions. Indeed, in [7–9], Aiki and Muntean consider a system of reaction–diffusion equations on a moving domain describing concrete carbonation. In this case, only one boundary is free and there is no steady-state: they prove that the thickness of the domain increases following a $\sqrt{t}$-law.

1.2. Presentation of the DPCM model

The DPCM model was introduced in [1]. It consists of three drift–diffusion equations for the densities of charge carriers – ferric cations (P), electrons (N) and oxygen vacancies (C) –, coupled with one elliptic equation for the electric potential (Ψ) and two evolutive equations for the interfaces of the domain (X_0, X_1).

We consider here the dimensionless DPCM model. We will first present the equations and then give a sense to all the parameters involved in the equations. Let us mention that the scaling in time is performed with respect to the characteristic time of the cations. The equations for the carrier densities P, N, C, as the boundary conditions, have the same form. For $U = P, N$ or C, they are written:

$$\varepsilon_U \partial_t U + \partial_x J_U = 0, \qquad J_U = -\partial_x U - z_U U \partial_x \Psi \quad \text{in } (X_0(t), X_1(t)), \forall t \geq 0, \tag{1a}$$

$$-J_U + U X_0'(t) = r_U^0(U(X_0(t)), \Psi(X_0(t))) \quad \text{on } x = X_0(t), \forall t \geq 0, \tag{1b}$$

$$J_U - U X_1'(t) = r_U^1(U(X_1(t)), \Psi(X_1(t)), V) \quad \text{on } x = X_1(t), \forall t \geq 0, \tag{1c}$$