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Mathematical model for acid water neutralization with anomalous and fast diffusion


 A. Ceretani^{a,b,*}, J. Bollati^{a,b}, L. Fusi^c, F. Rosso^c
^a Conicet-Universidad Austral, Paraguay 1950, S2000FZF, Rosario, Argentina

^b Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Pellegrini 250, S2000BTP Rosario, Argentina

^c Dipartimento di Matematica e Informatica “U.Dini”, Università degli Studi di Firenze, Viale Morgagni 67/a, 50134 Firenze, Italy

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ABSTRACT

In this paper we model the neutralization of an acid solution in which the hydrogen ions are transported according to Cattaneo’s diffusion. The latter is a modification of classical Fickian diffusion in which the flux adjusts to the gradient with a positive relaxation time. Accordingly the evolution of the ions concentration is governed by the hyperbolic telegraph equation instead of the classical heat equation. We focus on the specific case of a marble slab reacting with a sulphuric acid solution and we consider a one-dimensional geometry. We show that the problem is multi-scale in time, with a reaction time scale that is larger than the diffusive time scale, so that the governing equation is reduced to the one-dimensional wave equation. The mathematical problem turns out to be a hyperbolic free boundary problem where the consumption of the slab is described by a nonlinear differential equation. Global well posedness is proved and some numerical simulations are provided.

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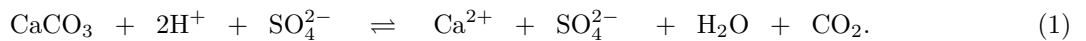
1. Introduction

When sulphide minerals present in rocks are exposed to air and water, sulphuric acid is produced as a consequence of a chemical reaction. The acidic water flow is known as Acid Rock Drainage (ARD). Though this is a natural process, it is highly enhanced by mining activities and it is then known as Acid Mine Drainage (AMD). AMD can cause serious damage in biodiversity and human health, especially after a mine plant has ended its activity. So treatment of acid water becomes a challenge in order to avoid long term environmental damage. A survey on remediation options for AMD can be found in [1]. The main techniques are based on chemical reactions neutralizing the acid water. A typical approach is the so-called limestone neutralization, which consists in the addition of a calcium carbonate base to the acidic water in order to reduce the acidity of the solution. In the last few years several models have been developed to describe the

* Corresponding author at: Conicet-Universidad Austral, Paraguay 1950, S2000FZF, Rosario, Argentina.
E-mail address: aceretani@austral.edu.ar (A. Ceretani).

evolution of this sort of neutralizing systems [2–5]. Although these models were proposed taking into account different aspects of the diffusive–reactive process, all of them are based on Fick’s law (classical diffusion). When using Fick’s law, it is tacitly assumed that local disturbances are spread infinitely fast throughout the solution. This is a clear idealization and it is physically unrealistic, giving rise to the pathological feature of infinitely fast spreading of perturbations in the diffusion equation. For this reason, Cattaneo and others have proposed to modify Fick’s law in a way such that the flux may adjust to the gradient with a small but nonzero relaxation time, see [6].

In this article we study the evolution of a neutralization process for an acid solution in which transport is driven by Cattaneo’s law (anomalous diffusion). Following [5], we consider the reaction occurring between a sulphuric acid solution (H_2SO_4) and a slab of marble, which is mainly formed by calcium carbonate (CaCO_3):



The H_2SO_4 dissolved in the aqueous solution is dissociated in ions SO_4^{2-} and 2H^+ , where the concentration of the latter is commonly measured through the so-called pH. The acid reacts with CaCO_3 liberating Ca^{2+} ions in the solution. As the reaction takes place, the CaCO_3 is consumed and the concentration of H^+ ions decreases (the pH is hence raised). When the pH reaches a value around 7 the solution is said to be neutral and the reaction ceases. The reaction between H_2SO_4 and CaCO_3 takes place on the contact surface that separates the solid and the solution. From (1) we see that the stoichiometric ratio in the reaction between H^+ ions and CaCO_3 is 2:1, which means that two moles of H^+ are neutralized by one mole of CaCO_3 . Moreover the reaction is of first order, so that the exponents of the concentrations appearing in the rate equation are equal to 1. When other reactants and/or acid solutions are used, different ratios and different reaction orders may occur. Here, differently from [5], we do not consider the phenomenon of “armoring”, that consists in the formation of a thin coat of material on the reacting surface which partially or completely inhibits the reaction.

In this paper we model a system consisting in a rectangular container filled with sulphuric acid where a slab of marble has been placed on the bottom. This slab is assumed to occupy less than the half of the container height at the beginning. We also assume that the container is large enough, so that the system can be described in a one dimensional geometry¹ $[0, L^*]$ where the solid occupies a region $[0, s^*]$, the liquid fills the region $[s^*, L^*]$, with s^* evolving with time.

We study the system for the evolution of both the H^+ concentration and the reacting surface s^* . We assume that no acid is added or removed during the process and we notice that our system is physically consistent only if $\dot{s}^* < 0$ (the solid slab can only be consumed). The transport of H^+ in the solution is governed by Cattaneo’s diffusion and the nature of the mathematical problem is therefore hyperbolic. The system is multi-scale in time with three characteristic times: (i) the characteristic diffusive time; (ii) the relaxation time; (iii) the reaction time. Depending on the order of magnitude of these times different problems may arise. In particular, following [7] we show that the reaction scale is larger than the diffusion time scale, so that the consumption of the marble slab is slower than the diffusive transport of H^+ ions. Assuming that the relaxation time is sufficiently large we prove that the mathematical problem can be simplified to one in which the governing equation is the one dimensional wave equation. Following [8] we determine representation formulas for the solution that allow to write the evolution of the free boundary s^* as an implicit nonlinear differential equation. Global existence and uniqueness are proved. Finally numerical simulations that illustrate the behavior of the solution s^* and the dependence on the physical parameters of the problem are provided.

¹ Throughout the paper the starred quantities denote dimensional quantities.

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