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A fast precipitation and dissolution reaction for a reaction–diffusion system arising in a porous medium[☆]

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Abstract

This paper is devoted to the study of a fast reaction–diffusion system arising in reactive transport. It extends the articles [R. Eymard, T. Gallouët, R. Herbin, D. Hilhorst, M. Mainguy, Instantaneous and noninstantaneous dissolution: Approximation by the finite volume method, ESAIM Proc. (1998); J. Pousin, Infinitely fast kinetics for dissolution and diffusion in open reactive systems, Nonlinear Anal. 39 (2000) 261–279] since a precipitation and dissolution reaction is considered so that the reaction term is not sign-definite and is moreover discontinuous. Energy type methods allow us to prove uniform estimates and then to study the limiting behavior of the solution as the kinetic rate tends to infinity in the special situation of one aqueous species and one solid species.

Keywords: Reaction–diffusion; Precipitation; Dissolution; Kinetics; Fast reaction

1. Introduction

In this paper we consider the reaction–diffusion system,

$$(\mathrm{P}^\lambda)\quad \begin{cases} u_t = \Delta u - \lambda G(u, w) & \text{in } \Omega \times (0, T) \quad \text{(a)} \\ w_t = \lambda G(u, w) & \text{in } \Omega \times (0, T) \quad \text{(b)} \\ \dfrac{\partial u}{\partial n} = 0 & \text{on } \partial\Omega \times (0, T) \quad \text{(c)} \\ u(x, 0) = u_0(x), \qquad w(x, 0) = w_0(x) & \text{for } x \in \Omega, \quad \text{(d)} \end{cases} \tag{1.1}$$

where Ω is a bounded domain in $\mathbb{R}^N$ with smooth boundary $\partial\Omega$ and T is a positive constant. We suppose that λ is a positive constant and that the function $G(\cdot, \cdot)$ is given by

$$G(u, w) = (u - \overline{u})^+ - \mathrm{sign}^+(w)(u - \overline{u})^-, \tag{1.2}$$

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where $\overline{u}$ is a given positive constant and

$$s^+ = \max(0, s), \qquad s^- = \max(0, -s), \quad \text{and} \quad \operatorname{sign}(s) = \begin{cases} 1 & \text{if } s > 0, \\ -1 & \text{if } s < 0, \\ 0 & \text{if } s = 0. \end{cases}$$

The above system (P^λ) is a simplified adimensional model of reactive transport in a porous medium at the Darcy scale, where u stands for a concentration of an aqueous species, therefore mobile, and w stands for a concentration of a mineral species. The term $\lambda G(u, w)$ is a reaction rate that models either a precipitation if $u - \overline{u} \geq 0$, or a dissolution otherwise. The positive constant $\overline{u}$ is the thermodynamic constant of the dissolution reaction and λ is a constant rate. Reactive transport problems arise in the field of radioactive waste storage, oil industry or CO_2 storage. Indeed, water–rock interactions like precipitation and dissolution reactions have a strong impact both on flow and solute transport.

We focus on reactions which are very fast compared with the diffusion process so that λ is a large parameter. In this paper we extend a result of Eymard, Hilhorst, van der Hout and Peletier [6], which they obtained in the special case of a function $G(\cdot, \cdot)$ assumed to be nonnegative and nondecreasing in both arguments. This special assumption led to an easy way for estimating the time derivative of w in L^1 independently of λ. The Stefan problem obtained when $\lambda \to +\infty$ is the same as that of [7,11] but the problem (P^λ) considered in this paper has an additional precipitation term which prevents $G(\cdot, \cdot)$ from keeping a constant sign, and has led us to provide an original estimate. In [7], the main tool is a finite volume method used in any space dimension. In [11], a Legendre function (associated with the liquid concentration) is used in one-space dimension to deal with discontinuities. Note that in [3], the existence of a solution to the same problem with two aqueous species instead of one is proven; however, the study of the singular limit in this more complex case is still an open problem, since the techniques presented here do not seem to be easily adaptable. We suppose that the initial functions u_0 and w_0 satisfy the hypotheses:

$$(\mathrm{H}_0) \quad \begin{cases} u_0, w_0 \in L^2(\Omega) \quad 0 \leq u_0 \leq M_1 \text{ and } 0 \leq w_0 \leq M_2 \text{ a.e in } \Omega, \\ \text{for some positive constants } M_1 \text{ and } M_2 \text{ such that } M_1 > \overline{u}. \end{cases}$$

We set $Q_T := \Omega \times (0, T)$ and denote by $W_2^{2,1}(Q_T) = \{u \in L^2(Q_T), \frac{\partial u}{\partial x_i}, \frac{\partial^2 u}{\partial x_i \partial x_j}, \frac{\partial u}{\partial t} \in L^2(Q_T), i, j = 1, \ldots, N\}$ and by $C^{0,1}([0, T]; L^\infty(\Omega))$ the space of Lipschitz continuous functions with values in $L^\infty(\Omega)$. Next we define a notion of weak solution for Problem (P^λ).

Definition 1.1. (u^λ, w^λ) is a weak solution of Problem (P^λ) if for all $T > 0$

(i) $u^\lambda \in W_2^{2,1}(Q_T),\ w^\lambda \in C^{0,1}([0, T]; L^\infty(\Omega))$;
(ii) $\int_\Omega u^\lambda(T)\xi(T) - \int_\Omega u_0\xi(0) - \int_{Q_T} \left\{u^\lambda \xi_t - \nabla u^\lambda \nabla \xi - \lambda G(u^\lambda, w^\lambda)\xi\right\} = 0,$
$\int_\Omega w^\lambda(T)\xi(T) - \int_\Omega w_0\xi(0) - \int_{Q_T} \left\{w^\lambda \xi_t + \lambda G(u^\lambda, w^\lambda)\xi\right\} = 0,$
for all $\xi \in H^1(Q_T)$.

In view of its regularity, we remark that it satisfies the differential equations in Problem (P^λ) a.e. in Q_T. The purpose of this paper is to prove the following result.

Theorem 1. *Suppose that u_0 and w_0 satisfy the hypotheses* (H_0)*. Then for every $\lambda > 0$, Problem* (P^λ) *has a unique nonnegative weak solution (u^λ, w^λ). Moreover there exist functions $U \in L^2(Q_T)$, $W \in L^2(Q_T)$ such that u^λ and w^λ converge strongly in $L^2(Q_T)$ to U and W respectively, as λ tends to ∞. The function $Z := -(U + W) + \overline{u}$ is the unique weak solution of the Stefan problem*

$$(\mathrm{SP}) \quad \begin{cases} Z_t = \Delta(Z^+) & \textit{in } \Omega \times (0, T) & \text{(a)} \\ \dfrac{\partial Z^+}{\partial n} = 0 & \textit{on } \partial\Omega \times (0, T) & \text{(b)} \\ Z(x, 0) = -(u_0(x) + w_0(x) - \overline{u}) & \textit{for } x \in \Omega. & \text{(c)} \end{cases} \tag{1.3}$$

Conversely the limit pair (U, W) is given by $(U, W) = (\overline{u} - Z^+, Z^-)$.

This paper is organized as follows : In Section 2, we present a physical derivation of (P^λ). In Section 3, we prove a comparison principle for Problem (P^λ), which implies the uniqueness of its weak solution. This result is quite natural