Towards a thermodynamically consistent model for the corrosion of iron

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The derivation of models for the corrosion of iron that are accurate in the long-time regime is a challenge of great importance in many contexts, among which the management of nuclear wastes. This motivated many previous contributions. Our starting point here is the so-called Diffusion Poisson Coupled Model (DPCM) introduced in [1, 2], which describes the evolution of a magnetite layer separating a block of metallic iron from an aqueous domain. The derivation of the DPCM proposed in [1] does not rely on energetic considerations. As a consequence, its thermodynamic stability is unclear and neither a satisfactory well-posedness result nor the assessment of the long-time behavior of the system have been established so far.

In this project, we explore some as minor as possible corrections to make the DPCM free energy diminishing. We illustrate our approach on a simplified model inspired from the one studied in [3], where only two chemical species (electrons and iron cations) are assumed to be transported in a fixed and oxide layer due to chemical and self-consistent electrostatic effects. A special attention is paid to the boundary conditions at the interfaces between the oxide and the metal and between the oxide and the solution. We propose a global existence result following the methodology introduced in the seminal contributions of Gajewski and Gröger [4]. In opposition to what was established in [3], our result does not require any compatibility condition on the physical coefficients, as a consequence of the nonlinear stability of our system inherited from thermodynamics.

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