Post-doc (12 months) – Variational models for corrosion: mathematical modeling and numerical analysis

General context. Materials play a key role in the energy transition. The fine understanding of their chemistry and physics is of paramount importance for the development of cutting edge technologies in the domain of batteries, solar plants or fuel cells. Modeling also plays a crucial role to assess the aging of materials, like for the corrosion of metal or alloys. In sensitive applications, like for instance for the management of nuclear plants or of nuclear waste repositories, a fine description of the corrosion phenomena is required beyond state of the art models. In collaboration with colleagues from CEA and ANDRA, important efforts have been carried out during the last 15 years to derive and to simulate models representing the evolution of the thin oxide layer protecting the iron canister containing long-life radioactive wastes [1, 2]. Due to the lack of mathematical structure of the models, only partial mathematical results have been established so far.

Recent advances. Building on new developments in the field of generalized gradient flows, C. Cancès, C. Chainais-Hillairet, and collaborators work on the development of mathematical models of dissipative nature for the description of the oxide layer accounting for the evolution along time of the geometry. Preliminary results [3, 4] show that the corresponding model behaves better than previously existing ones. A prototype numerical code has been developed in Python to approximate the solution of the new model. Numerous challenges remain, and we propose to address some high impact open questions related to the mathematical modeling and the numerical analysis of dissipation driven corrosion models.

Research program. There is, so far, no theoretical foundations for the model involving mobile free boundaries proposed in [4], besides the fact that the model encodes the second principle of thermodynamics and has a Lyapunov functional. The rigorous proof of the existence of a weak solution in part of an ongoing study. The following questions should be addressed by the post-doc to be hired in the ANEDP team of the Laboratoire Paul Painlevé (Univ. Lille, CNRS), who will also be part of the Inria RAPSODI project team.

- Investigate the long-time behavior of the solution, and in particular the convergence of the solutions to the continuous model towards travelling wave profiles.
- Perform the numerical analysis (existence of discrete solutions, convergence as the grid size and the time step go to 0, ...) of the thermodynamically consistent finite volume scheme implemented in our prototype code.
- Investigate the long-time behavior of the approximate solution provided by the finite volume scheme, and establish its convergence towards a discrete travelling wave profile.

Informations. The future post-doc will be recruited by the French center for scientific research (CNRS) to start a 12 month contract in January 2025. If you are interested in the position, please contact Clément Cancès and/or Claire Chainais-Hillairet for further informations.

References

[1] C. Bataillon, F. Bouchon, C. Chainais-Hillairet, C. Desgranges, E. Hoarau, F. Martin, S. Perrin, M. Tupin, and J. Talandier. Corrosion modelling of iron based alloy in nuclear waste repository. *Electrochimica Acta*, 55(15):4451–4467, 2010.

[2] C. Bataillon, F. Bouchon, C. Chainais-Hillairet, J. Fuhrmann, E. Hoarau, and R. Touzani. Numerical methods for the simulation of a corrosion model with moving oxide layer. *J. Comput. Phys.*, 231(18):6213–6231, 2012.

[3] C. Cancès, C. Chainais-Hillairet, B. Merlet, F. Raimondi, and J. Venel. Mathematical analysis of a thermodynamically consistent reduced model for iron corrosion. *Z. Angew. Math. Phys.*, 74(96), 2023.

[4] C. Cancès, C. Chainais-Hillairet, B. Merlet, F. Raimondi, and J. Venel. Thermodynamically consistent modelling of the corrosion of iron in the context of deep subsurface nuclear waste repositories. HAL: hal-04210782, 2023.