

Title: Modeling coupled transport processes through semi-permeable membranes with a reactive transport modeling approach

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Host University	University of Orléans
Main site	Orléans
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Summary

A membrane is a semi-permeable barrier which permits the transport of some components of a solution and not others. A membrane rejects solutes on the basis of size and/or electrical restrictions. In the second case, it can give rise to electroosmosis, hyperfiltration and chemical osmosis processes (the so-called off-diagonal terms), as a result of coupled transport processes between pressure, electrical and chemical gradient. Various Darcy scale models describing water and ion transport in charged media have been proposed in the literature that rely on the description of a representative elementary volume by volume averaging, and where off-diagonal terms are treated using phenomenological coefficients. However, these approaches were mostly restricted to cases where (i) the solution composition was described by a symmetric electrolyte, and where (ii) the porosity could be assimilated to a homogeneously charged domain with average properties. These restrictions have many limitations. These identified restrictions can be overcome with an advanced reactive transport modeling approach that we have developed. The objective of the thesis is thus to implement and then use such an approach in two different contexts: containment of contaminants by clay barriers, and water treatment using reverse osmosis. The work of the Ph.D. student will be mainly focused on developing theoretical aspects and testing numerical implementations of the off-diagonal terms, in order to prepare their full implementation in the reactive transport code CrunchClay.

Keywords: membrane, reactive transport, coupled processes

Candidate Profile

We are seeking a student with a master degree in Earth Sciences, Civil Engineering, Physics or Chemistry, with a strong background in geochemistry, hydrology and/or computational methods. The candidate should be motivated by theoretical and numerical research work. The candidate should be independent in his/her work and should have a rigorous approach of scientific issues. This Ph.D. position requires also international mobility because part of the work will be carried out at the Lawrence Berkeley National Laboratory, Berkeley, California, USA in the framework of the Memorandum of Understanding signed by BRGM and LBNL.

Expected Starting date: October 2019. Review of applications will begin May 1, 2019 and will continue until the position is filled.

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