

COUPLED MULTI-PHYSICS SIMULATION IN ELECTRODIALYSIS FOR SEA WATER DESALINATION

K. Masilamani^{1,2*}, J. Zudrop², H. Klimach² and S. Roller²

¹ Siemens AG, Corporate Technology, CT RTC ENC ENT-DE, Günther-Scharowsky-Str. 1,
91058 Erlangen, Germany

² Simulation Techniques and Scientific Computing, Hölderlinstr. 3, 57068 Siegen, Germany,
kannan.masilamani@uni-siegen.de, j.zudrop@grs-sim.de, harald.klimach@uni-siegen.de,
sabine.roller@uni-siegen.de. <http://www.mb.uni-siegen.de/sts>

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The development of an efficient sea water desalination technique to supply mankind with clean drinking water is a major challenge today. Electrodialysis is an energy and cost efficient technique in comparison to more conventional techniques. In this process, ion exchange membranes are used to separate salt ions from sea water with the help of an applied external electrical field. Electrodialysis is complex and involves the interaction of several different physical phenomena. To optimize this process, a better understanding must be acquired by gaining insight into the involved effects. Currently, this is only achievable by large-scale coupled numerical simulations. In this work we present our approach to address the simulation of the complete process.

An electrodialysis module consists of selective ion exchange membranes, the anion and cation exchange membranes, which are arranged alternately and allows only anion and cations to pass through, respectively. A complex net like structure, called the spacer, is used as a mechanical stabilizer to keep the membranes apart from each other. The spacer has an influence on the transport of ions through membranes and on the overall pressure drop of the flow channel. Due to charged ions, the electro-magnetic fields are altered and in turn the driving forces on the ions vary accordingly. To cover these effects, a strongly coupled numerical simulation of electro-magnetic fields and the ion transport is required.

To model the transport of ionic species and mixture in the flow channel, the multi-species Lattice Boltzmann Method (LBM) [1] is used. This method is chosen as our numerical scheme due to its advantage in incorporating complex geometries and its high performance on large scale supercomputing systems. In the macroscopic limit, this method recovers the Navier-Stokes equations with external forces for mixtures and the Maxwell-Stefan equations for ion transport with external forces. A Discontinuous Galerkin (DG) method

is used to simulate the electro-magnetic fields, described by the Maxwell equations. This method is chosen for this part, due to its high locality and low numerical dissipation, provided by the high order of the scheme.

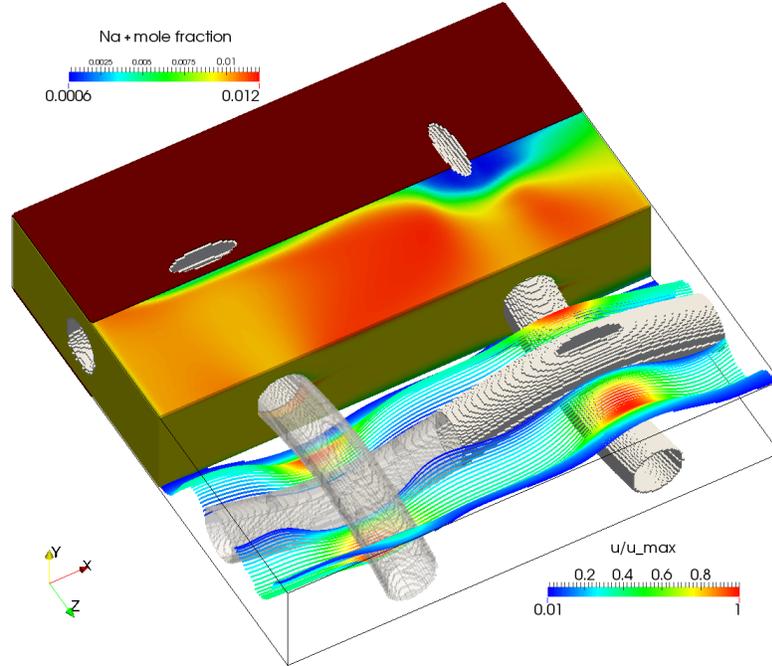


Figure 1: Concentration profile of Na+ ion shows higher concentration at $y=Height$ due to applied external electrical field in y -direction. Stream lines indicate the mixture flow in x -direction

The multi-species LBM is implemented in our highly scalable LBM solver MUSUBI [2] and coupled with our DG solver Ateles which are part of our octree based parallel simulation framework APES [3]. The steps involved in the coupling these two numerical schemes and results obtained for the specific application for desalination are detailed. The concentration profile of ion transport with a spacer structure in the flow channel and an external electrical field perpendicular to the flow direction is shown in Figure 1. The investigation of various parameters like flow velocity, external electrical field and spacer design effects on the transport of salt ions are investigated.

REFERENCES

- [1] J. Zudrop, S. Roller and P. Asinari. A Lattice Boltzmann Scheme for Liquid Mixtures - Part I: Model and Analysis. *Physical Review E* (2013) (Under review)
- [2] M. Hasert, K. Masilamani, S. Zimny, H. Klimach, J. Qi, J. Bernsdorf, S. Roller. Complex Fluid Simulations with the Parallel Tree-based Lattice Boltzmann Solver. *J. Comput. Sci.* (2013), <http://dx.doi.org/10.1016/j.jocs.2013.11.001>
- [3] S. Roller et al. An adaptable simulation framework based on a linearized octree. In *High performance computing on vector systems 2011*, Editors: M. Resch, X. Wang, W. Bez, E. Focht, H. Kobayachi, and S. Roller, Springer.