

Effective reactive ion transport under dominant flow conditions

Nadja Ray, Friedrich-Alexander-University Erlangen-Nürnberg,
Raphael Schulz, Friedrich-Alexander-University Erlangen-Nürnberg,
Kundan Kumar, University of Bergen

Key words: Taylor dispersion, electroosmotic flow, homogenization

Abstract

We consider a pore-scale model for reactive flow and transport of potentially charged species in a thin 2-D strip. Reactions leading to a non-negligible deposited layer on at the lateral boundaries of the strip lead to a free boundary value problem in which the moving interface between the fluid and the deposited (solid) layer is explicitly taken into account. Using asymptotic expansion methods, we derive an upscaled, one-dimensional model by averaging in the transversal direction. In doing so we focus on the cases, where the convective and/or electroosmotic transport dominate the diffusive transport. We highlight the difference and interplay of hydrodynamic dispersion (Taylor-Aris dispersion) and dispersion created by electroosmotic flow. The results are consistent with models known in the literature for a constant geometry and models in which either convection or electroosmotic effects dominate diffusion, cf. [1]. Finally, numerical computations are complementing the theoretical results.

We consider reactive ion transport under dominant flow conditions in a thin, potentially evolving, strip. At the pore-scale a fluid is flowing through the pore space of the porous medium and transports dissolved ions with concentrations c^\pm . Electric charges and an applied electric potential (zeta potential) give rise to electroosmotic flow in addition to pressure driven flow. As transport mechanisms we consider diffusion, convection, and electric drift. Additionally, chemical reactions of the type $c^+ + c^- \leftrightarrow c^{im}$ take place, with the resulting immobile component c^{im} being attached to or detached from the pore walls. Two distinctly different geometric situations are considered in this talk: In the first situation, we assume that the reaction product forms a very thin layer that does not influence the underlying geometry of the pore space. Alternatively, we assume that the thickness of the deposited layer is not negligible. Then the variations in the pore space and hence in the flow domain have to be taken into account. In this situation, the interface between the attached layer of immobile chemical species and the fluid is described via the thickness of the layer as has been done for reactive flows under dominant convection in [2]. In the case that diffusion dominates or is in balance with the pressure driven convective transport, the upscaling of the underlying model equations is well understood in both fixed and variable geometry frameworks. If the convective transport dominates the diffusion, it is well known that pressure driven flow leads to Taylor dispersion. In this talk, we focus on the impact of the applied electric potentials and the induced electroosmotic flow for the fixed geometry as well as for the evolving geometry. In this sense we consistently extend the results obtained in [2, 1]. We employ the asymptotic expansion method to derive the upscaled model equations.

First we consider the fixed geometry case. Additionally to an externally applied electric field we take into account a double layer potential on the upper and lower boundary of the thin strip. This leads to a distribution of ions near the boundary for which an condition of electroneutrality does not hold. The two differently induced electric fields have considerable different properties and the total electric field is created by superposition of both fields. The external electric potential is driven by the applied electric potential on the inflow and outflow boundary. It does only depend on the horizontal coordinate x and comes along with constant electric field. Contrarily, the electric potential being generated from the prescribed double layer potential and the non balancing distribution of the ions within the double layer results in a potential that does depend on the vertical coordinate y and has $\cosh(y)$ as a functional dependency, cf. [1]. The total concentrations are likewise separated in concentrations within the double layer and bulk concentrations. The double layer concentrations obey the Boltzmann distribution and have significant influence on the velocity field which further determines the transport of the bulk ion concentrations. Besides pressure driven dispersion electroosmotic induced dispersion effects are deduced throughout the upscaling.

Moreover, we consider reactive ion transport in the evolving geometry case under the influence of an externally induced electric field and additionally take into account a double layer potential. Opposed to the previous model, in this section a constant density ρ is used rather than the concentration of an immobile chemical species. Moreover the evolving boundary is parametrized via the thickness of the resulting boundary layer. However, a no-slip boundary condition is applied for the fluid velocity instead of a zero Dirichlet boundary condition. This means that the interface between the attached layer of immobile chemical species and the fluid moves with the same velocity as the boundary layer's growth rate. The divergence of the Darcy velocity equals

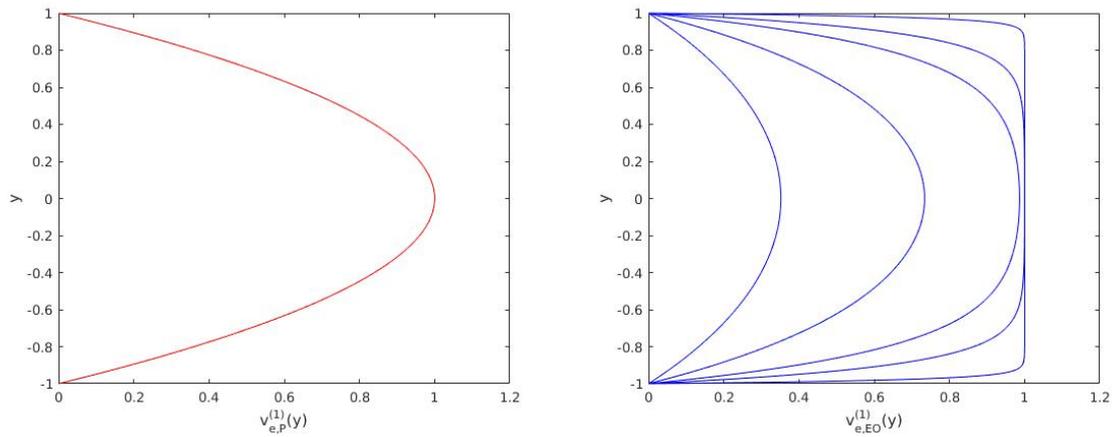


Figure 1: Profiles of the local velocity due to pressure driven flow (left) and electroosmotic flow (right) for different parameter $\kappa = 50, 10, 5, 2, 1$, cf. [1].

with the change of the thickness of the layer in time, i.e. the flow at the boundary is induced by the motion of the interface. This assumption is particularly reasonable for rapid interface movements (e.g. due to fast reactions or low densities of the attached layer). Moreover, particular attention is paid to the treatment of all electrically induced terms.

The strength of the applied method is that physically highly relevant dispersion relations are systematically derived - even for the evolving geometry. For specific situation, well known models including either Taylor dispersion or electroosmotic dispersion are reproduced. In our research we additionally reveal cross coupling dispersive effects and provide an explicit dependence of electroosmotic dispersive terms on the evolving geometry. The functional relations for electroosmotic flow and pressure driven flow indicate that electroosmotic flow induces a uniform flow field than pressure driven flow, cf. Figure 1. In this sense the rate of dispersion is significantly larger in the latter case. From the derivation of the effective model we conclude that the pressure driven and electroosmotic induced dispersion balance in the fixed geometry case. Contrarily, the degeneration of the terms including electroosmotic flow is significantly higher than the one including purely pressure driven dispersion for degenerating argument in the evolving geometry.

Finally, numerical computations for the different scenarios and different densities are performed to further illustrate the role of the two types of dispersion and the boundary layer.



Figure 2: Example of a figure

References

- [1] J.H. Maslyah and S. Bhattacharjee. *Electrokinetic and colloid transport phenomena*. John Wiley and Sons, Inc., Hoboken, New Jersey, ISBN: 978-0-471-78882-9, (2006).
- [2] K. Kumar, T.L. van Noorden and I.S. Pop. *Effective dispersion equations for reactive flows involving free boundaries at the microscale*, Multiscale Model. Simul. **9**(1), 29–58, (2011).
- [3] N. Ray and R. Schulz. *Derivation of an effective dispersion model for electroosmotic flow involving free boundaries in a thin strip*, Preprint Series Angewandte Mathematik 398, <http://www.math.fau.de/fileadmin/preprints/pr398.pdf>.