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A new efficient approach to solve the Nernst-Planck equation with a finite volume method

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Molecular diffusion of charged ions in heterogeneous media is an important process that determines migration rates of ions and is responsible for developing electric potentials in semi permeable membranes, biofilms and in charged porous media such as clays, soils and concrete.

To model such multicomponent diffusion processes an approach based on the Nernst-Planck equation is usually applied. This is considered computationally demanding, because in that case transport of individual chemical species is calculated, instead of the lumped transport of master species.

Furthermore the method has conceptual challenges in finite volume approaches with respect to correctly averaging cell/species properties of adjacent cells with contrasting mobility properties.

In correct implementation can lead to charge balance errors and subsequent numerical instabilities.

In this contribution we demonstrate an alternative approach, implemented in the ORCHESTRA framework, which has the following advantages:

- Transport properties of individual chemical species (and dependence on gradients in concentration, electric potential and activity) are summarized per master species.
- Only master / primary species need to be considered in the transport part.
- The required additional calculations are performed within the chemical solver, and are thus automatically parallelized.
- Within the transport part a zero (or given) charge flux condition is iteratively solved.
- The method can handle contribution of activity gradients on transport.
- The method automatically uses correct averaging between cells with different transport properties.
- The method prevents charge balance errors, which can arise when individual species are transported.

A comparison with literature benchmarks will be presented.

Implementation of the method in ORCHESTRA is relatively straightforward, as here it is possible to add the required additional calculations for chemical species as input for the chemical solver, and it is also possible to add the extra equation to be solved in the transport part without the need to change the source code. However, the method can be readily implemented in other codes.