Referee's Report on the manuscript egusphere-2022-1205

Po-Wei Huang, Bernd Flemisch, Chao-Zhong Qin, Martin O. Saar, and Anozie Ebigbo: *Validating the Nernst - Planck transport model under reaction-driven flow conditions using RetroPy v1.0*

The authors apply Nernst-Planck equation in order to model reactive transport processes in natural environment for single-phase multicomponent system. The importance of Nernst-Planck model is that it takes into account the electromigration of ionic species that have different diffusivities. On the other hand, if all species have the same diffusivity, the single-diffusivity model is obtained. For both models it is taken into account the electroneutrality condition and the zero-charge accumulation assumption.

The authors solve equations numerically. Mixed finite element method formulation in order to obtain fluid velocity and pressure is used. For the transport equation the authors have used finite volume scheme, in which they use upwinding for the advective flux, which is common approach in the equations for transport processes with convection and diffusion. For time-stepping they have used explicit scheme for advection term and Crank-Nicolson for the diffusion and the Nernst-Planck terms.

In this manuscript the results are presented for numerical experiments that deal with chemically driven convection of acid-base systems, and convective dissolution of CO_2 in reactive alkaline solutions. The authors compare the results of Nernst-Planck and single-diffusivity model mutually, and with experimental figures from the literature. Furthermore, in the last section authors discuss and explain on their obtained results.

I have found this manuscript very interesting. First numerical example is very interesting, and it provides the value of Nernst-Planck model. I recommend the manuscript for publication. The authors also provide a large amount of references about the topic of this manuscript. Furthermore all the simulations are obtained using RetroPy 1.0 that is available online.

In my opinion there are some minor points that are not clearly written:

- In Figure 1, a flow chart is represented. I suggest to use the same notation for the velocity as in the text of the manuscript

- Since the Nernst-Planck equation is non-stationary, for the sake of clarity, I suggest that you write the equation from which initial molar concentrations are obtained, to make everything mathematically more clearly, since for the boundary conditions no-flow boundary conditions are taken, the initial conditions must be written clearly.

- Could you please elaborate, how large is the system in (32) when you update the velocity, and explain the reason why you have chosen to solve it with direct solver? (Just to comment: since you have used direct solver for linear system (in which

possibly positive-definite matrix is added (rB^TB)) maybe you could try to use some iterative solver from PETSc, the library that was also used in this work for resolving nolinearity in transport equation)

- Could you please elaborate about the stepsizes Δt that have used in your simulations?