Referee's report on the paper

Validating the Nernst-Planck transport model under reaction-driven flow conditions using RetroPy v1.0

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The authors study the transport with electrodiffusion in continuous media, in the two-dimensional case, $2D$. They start with the continuity equations

$$\frac{\partial C_i}{\partial t} + \nabla \cdot J_i = 0, \quad i = 1, ..., N-1, \tag{1}$$

where C_i mean concentrations and the fluxes J_i are composed of three parts: Fick's part, Nernst-Planck's part an Darken's part as follows

$$J_i = -D_i \nabla C_i + \frac{z_i C_i D_i F}{RT} E + C_i u, \quad i = 1, ..., N-1. \tag{2}$$

Darken's velocity u fulfills Darcy's law

$$u = -\frac{k}{\eta}(\nabla p - \rho g) \tag{3}$$

and the incompressibility condition holds

$$\nabla \cdot (\rho u) = 0. \tag{4}$$

Under the electroneutral condition

$$\sum_{i=1}^{N-1} z_i C_i = 0, \tag{5}$$

the system (1) leads to the stationary equation

$$-\nabla \cdot \left(\sum_{i=1}^{N-1} \frac{D_i C_i (z_i F)^2}{RT} E - \sum_{i=1}^{N-1} D_i z_i F \nabla C_i \right) = 0. \tag{6}$$

The authors postulate, by the paper due to Tabrizinejadas et al., 2021, that the electric field has the form

$$E = \frac{RT \sum_{i=1}^{N-1} d_i z i \nabla C_i}{F \sum_{i=1}^{N-1} (z_i)^2 D_k C_k}. \tag{7}$$

Here is a very big mistake! The formula (7) is true in the 1D case only, if for example $\sum_{i=1}^{N-1} z_i J_i = 0$ on the boundary of a domain. Then (7) is implied by (6) - see the paper:
1. Bernard P. Boudreau, Filip J.R. Meysman, Jack J. Middelburg, *Multicomponent ionic diffusion in porewaters: Coulombic effects revisited*, Earth and Planetary Science Letters 222 (2004), 653-666.

Tabrizinejadas et al., 2021 study the 1D, 2D and 3D models and they refer to the paper 1., so they are right in 1D only. I understand that the authors get some pictures, but mathematics has its laws.

In 2D and 3D we can for example assume that E is an irrotational vector field, $\nabla \times E = 0$, and then E is a potential field

$$E = -\nabla\varphi. \tag{8}$$

This equation together with (6) imply the Poisson equation on φ of the form

$$\nabla \cdot \left(\sum_{i=1}^{N-1} \frac{D_i C_i (z_i F)^2}{RT} \nabla\varphi + \sum_{i=1}^{N-1} D_i z_i F \nabla C_i \right) = 0. \tag{9}$$

I refer the authors to the papers in which a similar situation appears, but with the drift u instead of the electric field E:

2. B. Bożek, L. Sapa, K. Tkacz-Śmiech, M. Zajusz, M. Danielewski, *Compendium about multicomponent interdiffusion in two dimensions*, Metallurgical and Materials Transactions A 52A (2021), 3221-3231.

3. L. Sapa, B. Bożek, K. Tkacz-Śmiech, M. Zajusz, M. Danielewski, *Interdiffusion in many dimensions: mathematical models, numerical simulations and experiment*, Mathematics and Mechanics of Solids 25 (2020), 2178-2198.

4. B. Bożek, L. Sapa, M. Danielewski, *Difference methods to one and multidimensional interdiffusion models with Vegard rule*, Mathematical Modelling and Analysis 24 (2019), 276-296.

The paper has an engineering and numerical nature, and is interesting. But the error I mentioned above must be reliably described and explained, even if the authors are currently unable to do calculations in 2D and 3D with the equation (9). I suggest to start with experiments and calculations in 1D. Moreover, the jump operator $[\bullet]$ should be defined and it would be better to write c_i instead of C_i. Domain dimension in experiments and calculations should be written in Abstract.

CONCLUSION
The paper need a major revision.