Referee’s report on the paper

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

Po-Wei Huang, Bernd Flemisch, Chao-Zhong Qin, Martin O. Saar, and Anozie Ebigbo

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

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

(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

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

(2)

Darken’s velocity $u$ fulfills Darcy’s law

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

(3)

and the incompressibility condition holds

$$\nabla \cdot (\rho u) = 0.$$  

(4)

Under the electroneutral condition

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

(5)

the system (1) leads to the stationary equation

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

(6)

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

$$E = \frac{RT \sum_{i=1}^{N-1} d_i z_i \nabla C_i}{F \sum_{i=1}^{N-1} (z_i)^2 D_i C_i}.$$  

(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:


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 \( \varphi \) 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 \( E \):


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.