Scaling for selectivity in uniformly charged selective nanopores

Zsófia Sarkadi, Dávid Fertig, Mónika Valiskó, Dezső Boda
Center for Natural Sciences, University of Pannonia, Egyetem str. 10., Veszprém, Hungary
sarkadi.zsofia@gmail.com

Nanopores are nanoscale channels embedded in a membrane providing a controlled transport of ions between the two bulk phases on the two sides of the membrane. The nanopore's radius, R, is in the nanometer range, comparable to the Debye length, λ_D.

Charge patterns are chemically deposited on the inner wall of the engineered nanopore providing different output signals for different input parameters. From the relation of the input and output signals a device function can be generated. In the case of a uniformly (negatively) charged nanopore, the device function is (cation) selectivity defined as $S_+ = I_+/I$ where I_+ is the cation current and I is the total current. The scaling of the selectivity of the nanopore means that selectivity is a unique smooth and monotonic function of the a well defined scaling parameter.

The scaling parameter is constructed from the input parameters of the nanopore device. We showed [1] that the Dukhin number [2] defined as

$$\mathrm{Du} = \sigma/eRc = \sigma 8\pi l_B \lambda_D^2/eR$$

is a suitable scaling parameter for the nanotube limit, namely, for the infinitely long nanopores ($H \to \infty$, where H is the length of the pore). In this formula, σ is the surface charge density and l_B is the Bjerrum length.

For the nanohole limit ($H \to 0$), we introduced [1] the modified Dukhin number defined as

$$\mathrm{mDu} = \mathrm{Du}\left(H/\lambda_D\right) = \sigma 8\pi l_B \lambda_D H/eR$$

and show that it is an appropriate scaling parameter. A mixed scaling parameter can be used in between.

We use simple models based on the primitive model of electrolytes and study those models with the Nernst-Planck (NP) transport equation coupled either to the Local Equilibrium Monte Carlo method (NP+LEMC) [3] or the Poisson-Boltzmann theory.

The latter, known as the Poisson-Nernst-Planck (PNP) theory, is a mean-field theory. We show that scaling is fundamentally a mean-field phenomenon. We show that the NP+LEMC and PNP results agree for 1:1 electrolytes where ionic correlations are weak, while deviations are found from the mean-field scaling behavior for 2:1 and 3:1 electrolytes. Thus, scaling can be considered as a measure of the applicability of mean-field theories.

REFERENCES

[1] Zs. Sarkadi, D. Fertig, Z. Ható, M. Valiskó, D. Boda, *J. Chem. Phys.,* **2021**, 154(15):154704.
[2] L. Bocquet and E. Charlaix, *Chem. Soc. Rev.*, **2010**, 39(3):1073-1095.
[3] D. Boda and D. Gillespie, *J. Chem. Theory Comp.,* **2012**, 10(8):824-829.

FIGURES

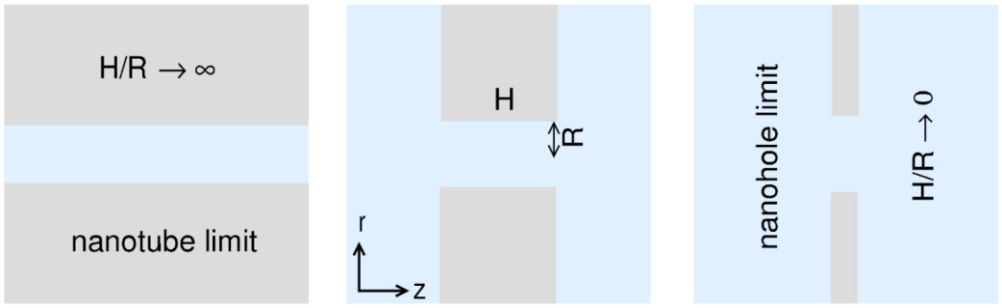

Figure 1: Pore geometries from the nanotube limit to the nanohole limit.