A 3D Poisson-Nernst-Planck study of the fluctuation driven transport in the OmpF channel

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In this work, the transport through the OmpF ion channel under electric potential fluctuations is analyzed numerically. Our goal is to determine under which conditions it is possible to obtain ion transport against its concentration gradient. To achieve this we use a model based on the 3D Poisson-Nernst-Planck transport equations, which allows us to obtain the flow of each ion under different conditions of concentration and applied potential, from the known three-dimensional structure of the OmpF pore (2OMF PDB access code).

Assuming that the system response under fluctuating potentials is determined by the I/V curve for each ionic species, it is possible to obtain the average current through the system. The results show that particularly high potentials would be required to achieve ion transport against its concentration gradient because of the low channel selectivity of OmpF and the relative inefficiency of the characteristic fluctuating signals of membrane cells [1]. We additionally compare the numerical results to experimental data to validate our approach.[2]

[1] M. Aguilella-Arzo, M. Queralt-Martín, M.-L. López, and A. Alcaraz, "Fluctuation-Driven Transport in Biological Nanopores. A 3D Poisson–Nernst–Planck Study," *Entropy 2017, Vol. 19, Page 116*, vol. 19, no. 3, p. 116, 2017.

[2] M. Lidón López, M. Queralt-Martín, and A. Alcaraz, "Stochastic pumping of ions based on colored noise in bacterial channels under acidic stress," *Nanoscale*, vol. 8, 2016.