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Using nanopores as sensors: a Monte Carlo modeling study

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We can distinguish natural (e.g., ion channels) and synthetic nanopores (e.g., carbon nanotubes, nanopores etched into plastic foils). The length of synthetic nanopores belongs to micrometer, while their radius belongs to the nanometer length scale. Ion transport through the nanopore has two main properties: rectification and selectivity. Due to these properties, the nanopore can be used as a rectifier diode or as a sensor. In this work, I examine the applicability of a nanopore as a sensor. We located binding sites inside the pore which are selective for the analyte, that is the molecule to be detected in the electrolyte filling the pore. Binding these particles to the nanopore's walls reduces the effective cross section of the nanopore, and, consequently, reduces the current carried by the main ions of the electrolyte through the pore. By measuring the drop of the current and constructing calibration curves, we can determine the concentration of the analyte.

In this modeling work, we create simple models the membrane, the pore, and the electrolyte. Negative charges are located on the cylindrical pore's wall to make the pore cation selective. For the electrolyte, the Primitive Model of electrolytes is used, which treats the ions as hard spheres with their charges located in the centers, and the solvent (water in this case) as a constant dielectric continuum. The binding sites are modeled with a square-well potential. The system is examined with the Local Equilibrium Monte Carlo (LEMC) method which is applicable for non-equilibrium systems. The currents of ions were calculated with the Nernst-Planck (NP) equation. This model and the method [1] (NP+LEMC) is suitable for examining low concentrations, that is important because the analyte is usually present in very small concentrations.

We examine the effect of various model parameters (for example, number, strength, and width of the binding sites; properties of the electrolyte and the analyte) on the sensitivity of the sensor by preparing calibration curves with different values of these parameters. Through the calculated concentration and potential profiles, the molecular mechanisms of the system can be observed well.

[1] D. Boda, D. Gillespie. *J. Chem. Theory Comp.*, **8**(3):824-829, 2012.