Surface Charge Modulated Ionic Conductance of Closed Solid State Nanopore Biosensors

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Introduction:

- Surface charge modulated ionic conductance effect in biomolecule detection by solid state nanopore biosensors is gaining importance.
- For open pore sensors, electrolyte flow rate adjustment is crucial for maximum binding, preventing such sensors from achieving a limit of detection below 1pg/ml.
- In closed silicon oxide nanoporous structure on silicon substrate, depletion layer capacitance at the pore bottom plays a major role in impedance sensing, enabling unique peak frequency based detection selective only to the target antigen.
- We aim to provide a framework for modelling the surface charge modulated ionic conductance in closed nanopores, which has not been reported earlier.

Results:

- Surface charge modulation effect is clear from the simulated potential profiles (fig.3)
- In order to compare the numerical results with a theoretical model, the potential profile in the pore has to be solved analytically.
- For that, we need to apply superposition theorem and sum up the two potential profiles (fig.4)
- Even ignoring edge effect at the pore entrance, i.e., the well-pore junction, there is a significant nonlinear dependence of current on pore length (fig.5), which can be exploited for the optimization of pore geometry, leading to performance enhancement.

Computational Methods:

- A closed pore is a cylinder terminated by a hemisphere having the same radius as the cylinder.
- Since in the steady state continuum regime, nanopore conductance is governed by the Poisson-Nernst Planck (PNP) equation, we have solved the 2D PNP equation using COMSOL.
- The Nernst Planck flux equations for each ionic species \( i \) is given by:
  \[ J_i = -D_i \nabla c_i \frac{z_i F}{RT} \nabla \phi \]
  where \( J_i \) is the flux of the \( i \)th species, \( D_i \) is its diffusion coefficient, \( z_i \) is its valence, and \( c_i \) is its concentration.
- The relationship between potential \( \phi \) and ionic concentration \( c_i \) is described by the Poisson equation:
  \[ \nabla^2 \phi = -\frac{F}{k_B T} \sum z_i c_i \]
- The equilibrium distribution of \( c_i \) follows a Boltzmann distribution given by:
  \[ c_i = c_{i,0} \exp \left( -\frac{z_i F \phi}{RT} \right) \]
- In order to solve the PNP equation, we have coupled ‘Electrostatics’ (Poisson equation) and ‘Transport of Diluted Species’ (Nernst Planck equation) physics.

Conclusions:

- Finite-element simulations demonstrate the role of surface charge in ion transport in closed nanopores.
- The results can be validated and compared by developing a proper analytical model.
- The two combined can provide a thorough understanding and analysis of the unexplored surface charge modulated ionic conductance in closed nanopores.

References:

3) X. Wang, S. Smirnov, ACS Nano 3, 4, 1004 (2009)