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.

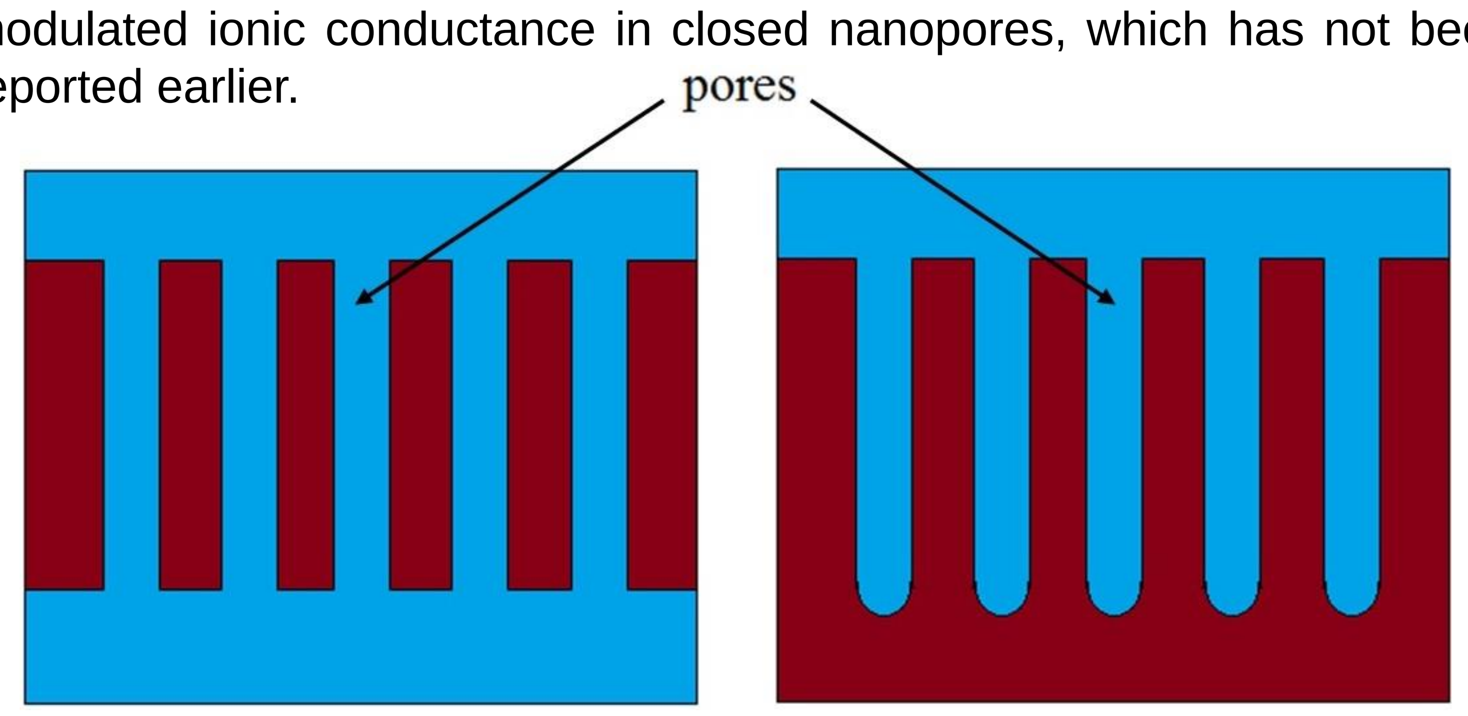

Fig.1a. Open Nanopore System **Fig.1b.** Closed Nanopore System

Computational Methods:

- A closed pore is a cylinder terminated by a hemisphere having the same radius as the cylinder.

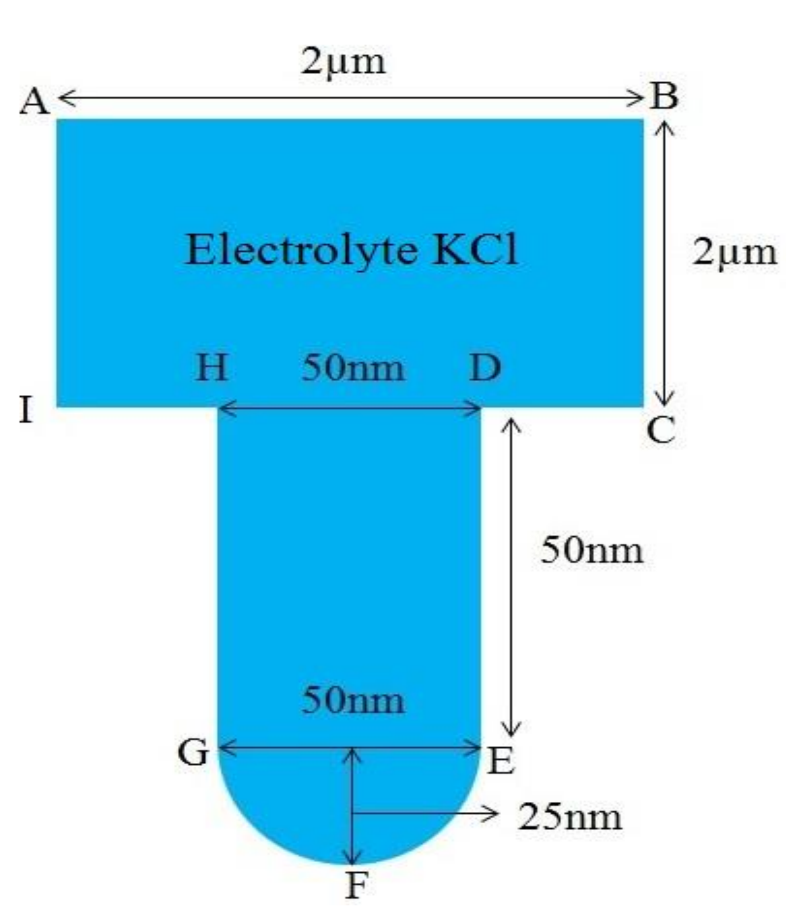

Fig.2. Geometry of the simulated structure (not to scale). ABCI represents the bulk electrolyte well and DEFGH represents the pore.

- 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

$$J_i = -D_i \nabla c_i - \frac{z_i F}{RT} D_i c_i \nabla \varphi$$

- The relationship between potential φ and ionic concentration c_i is described by the Poisson equation

$$\nabla^2 \varphi = -\frac{F}{\varepsilon\varepsilon_0} \sum_i z_i c_i$$

- The equilibrium distribution of c_i follows a Boltzmann distribution given by

$$c_i = c_{i,0} \exp\left(-\frac{z_i F \varphi}{RT}\right)$$

- In order to solve the PNP equation, we have coupled 'Electrostatics' (Poisson equation) and 'Transport of Diluted Species' (Nernst Planck equation) physics.

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.

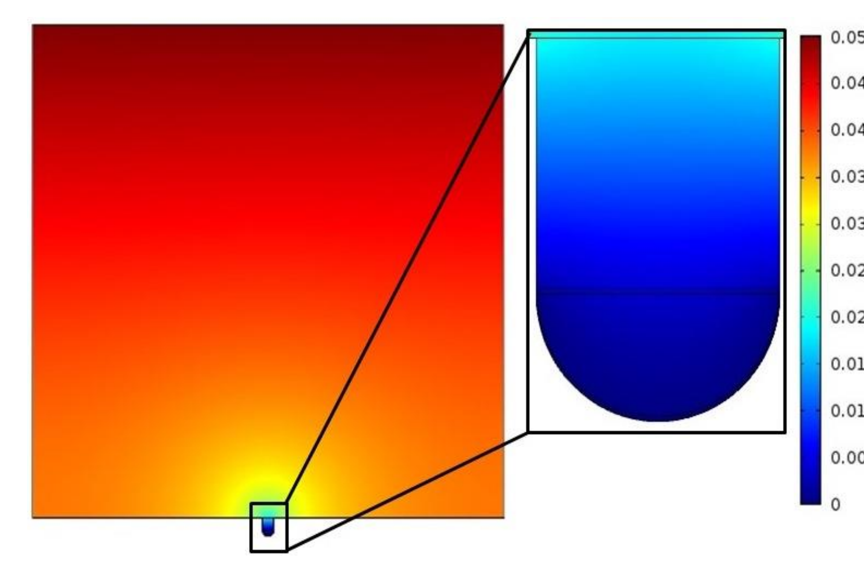

Fig.3a. Potential profile when no surface charge is applied

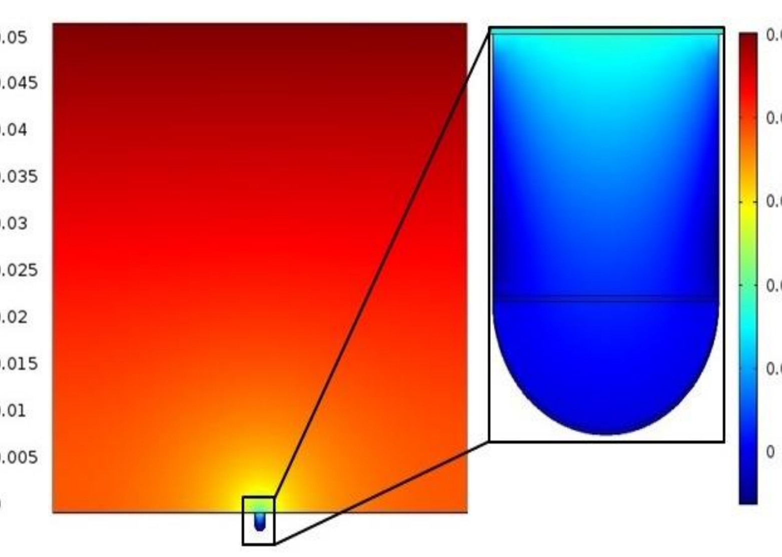

Fig.3b. Potential profile when surface charge is applied on both pore walls and pore bottom

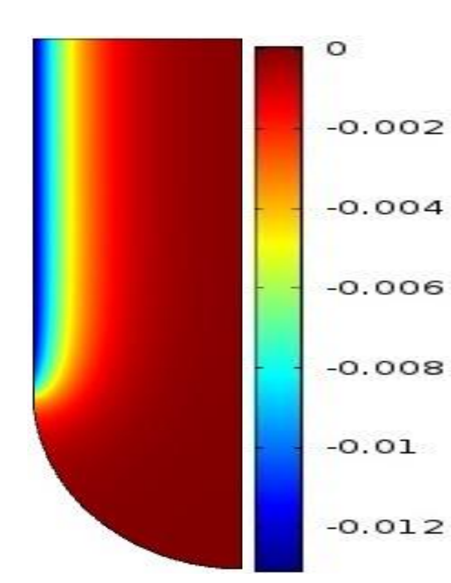

Fig.4a. Potential profile when surface charge is applied only on pore walls

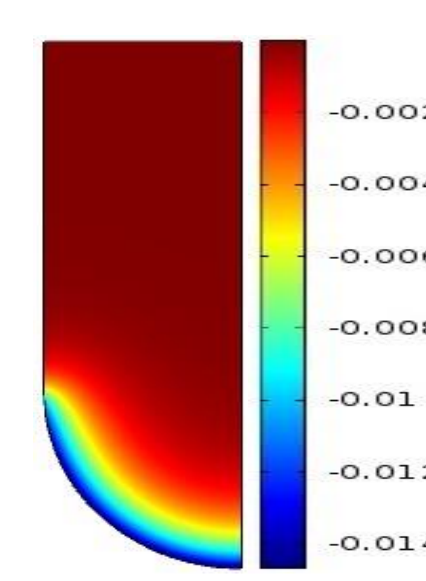

Fig.4b. Potential profile when surface charge is applied only on pore bottom

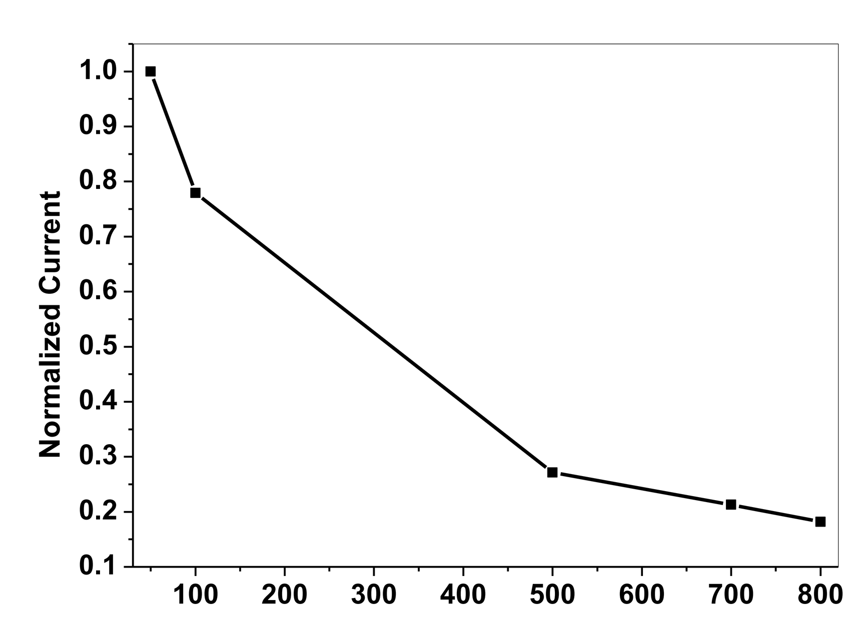

Fig.5. Normalized ionic current vs pore length for pore diameter = 50nm

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:

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