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The Contribution of the Electrical Double Layer to Enhance Ionic Currents in Single Walled Carbon Nanotubes.

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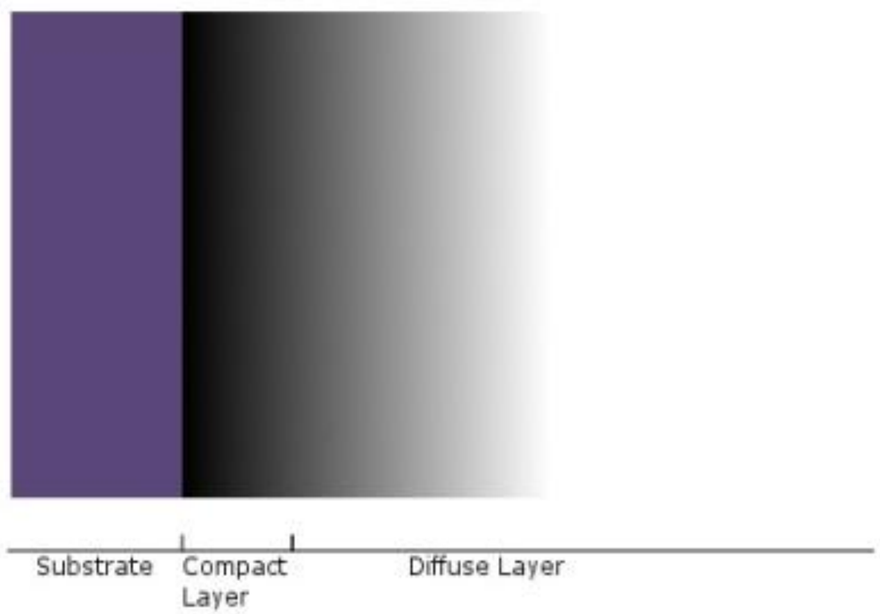
Enhanced Ionic Conductance in SWCNT

- Ionic conductance through SWCNT has been reported to be enhanced by 2 orders of magnitude
- Previous explanations have failed to account for all relevant phenomena at the nano-scale

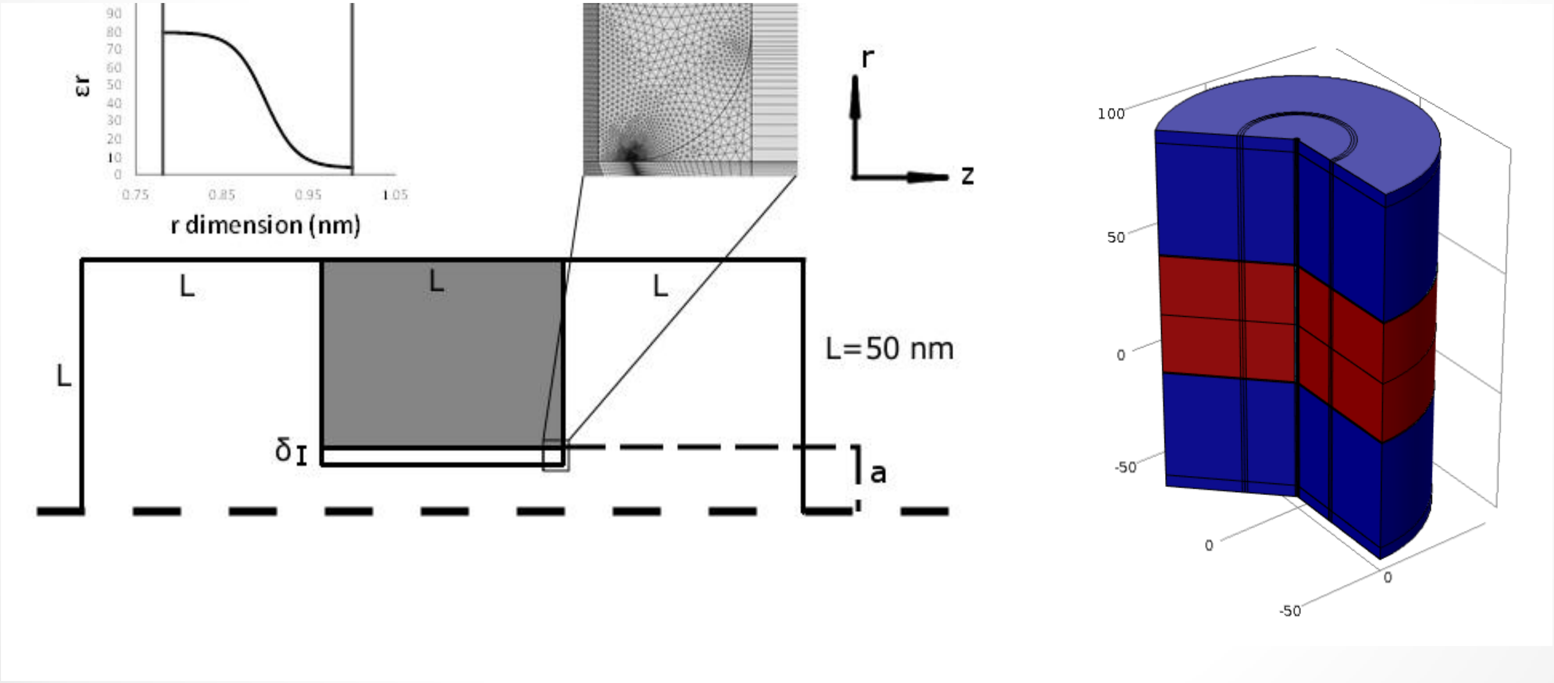
Electrical Double Layer

- An immobile compact layer forms at the surface due to electrical interactions between materials
- Mobile diffuse layer carries net charge



Model Geometry

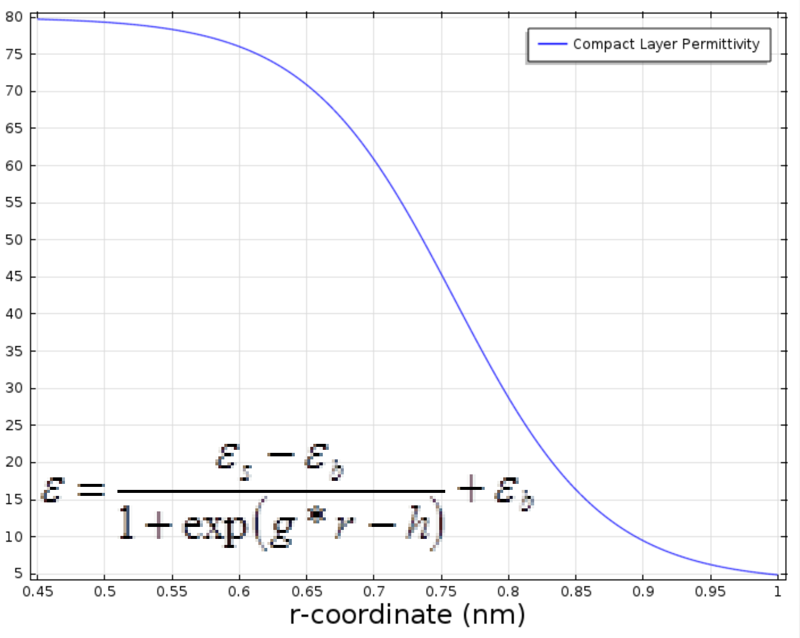
- SWCNT embedded in SiO_2
- 2D axisymmetric



The Compact Layer

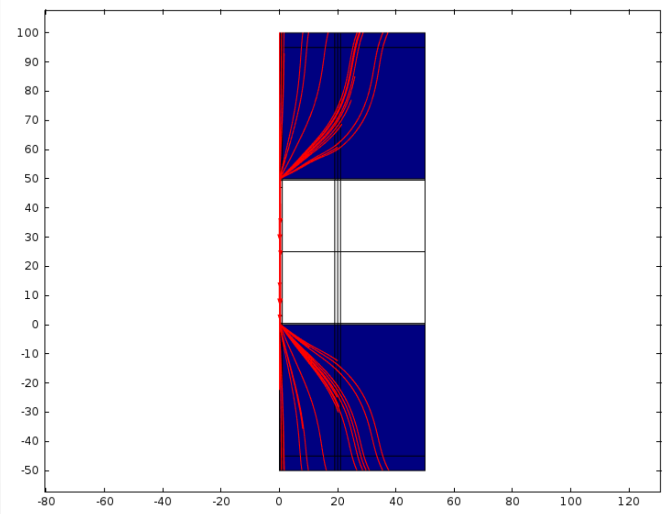
- A cylindrical shell at the interior surface of the SWCNT
- Smoothly varying permittivity

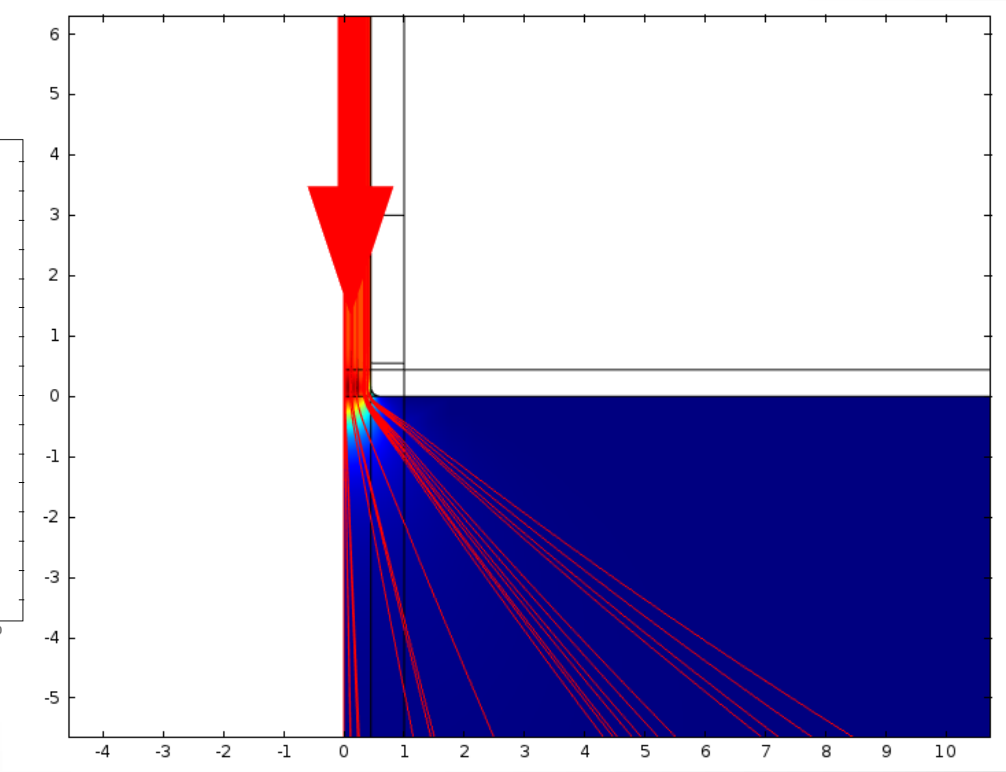
- Laplace Equation
  - $$\nabla^2 V = 0$$



The Compact Layer

- Slip at the outer Helmholtz plane
- Validated through observation and modeling
- Combined with the EDL, enables electroosmosis





Governing Equations

- Poisson Equation:
  - $$\nabla^2 V = -\frac{\rho(r,z)}{\varepsilon_0 \varepsilon_r}$$
- Accounts for material potentials, applied potentials, and ionic distributions

Governing Equations

- Nernst-Plank Equation:
    - $$\nabla \cdot (-D\nabla c - z\mu F c \nabla V) + u\nabla c = R$$
- Accounts for the transport of solvated ions via electrophoresis, electroosmosis, and diffusion

Governing Equations

- Stokes Equation:
  -

$$\rho(u\cdot\nabla)u=\nabla\cdot\left[-PI+\gamma\left\langle\nabla u+(\nabla u)^{T}\right\rangle-\frac{2}{3}\gamma(\nabla\cdot u)I\right]+F_{V}$$

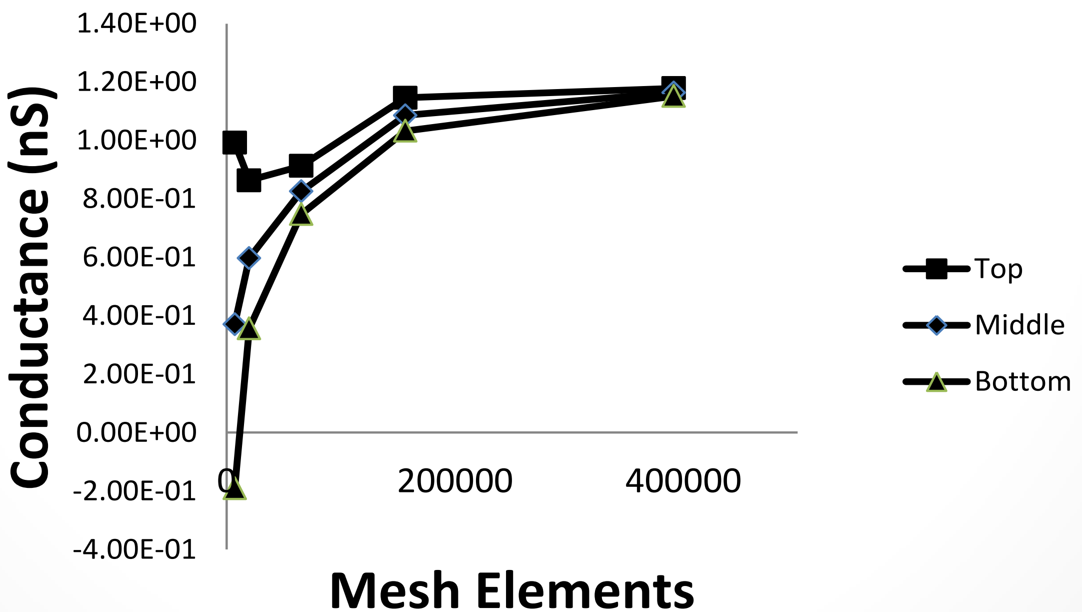
$$\nabla\cdot(\rho u)=0$$

- Accounts for the effect of a mobile solvent
  - Electroosmosis

$$\vec{F}_{V}=F_{c}\sum^{i}\left(z_{j}c_{j}\right)*E$$

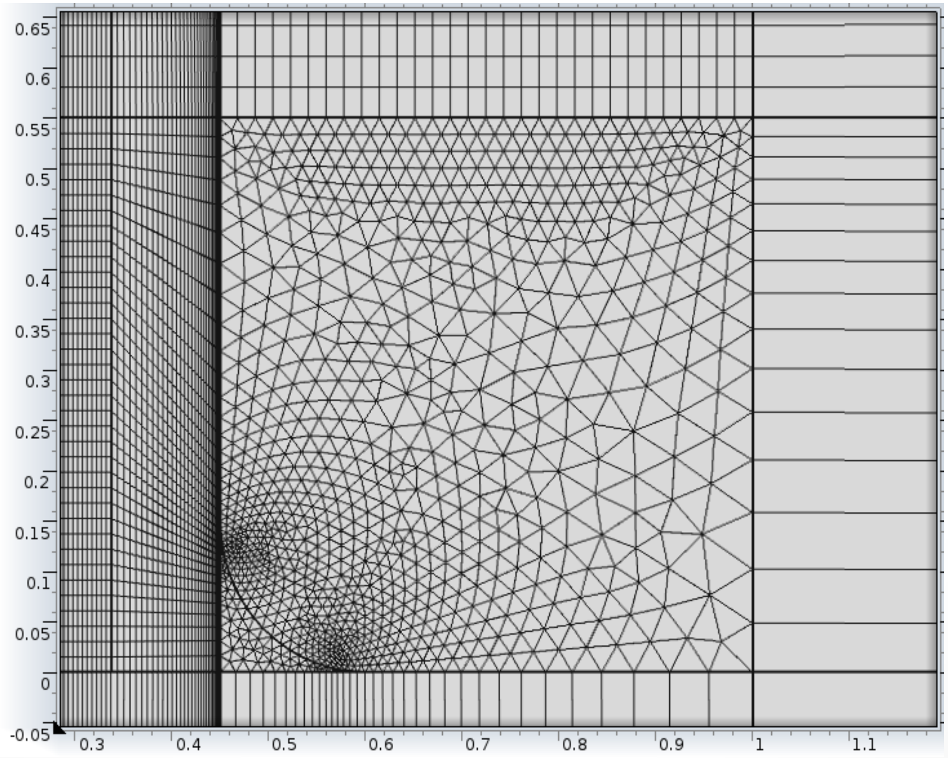
Mesh Convergence

- Iteratively refined until the conductance measured at the ends and middle of the channel were equivalent to 3 significant figures



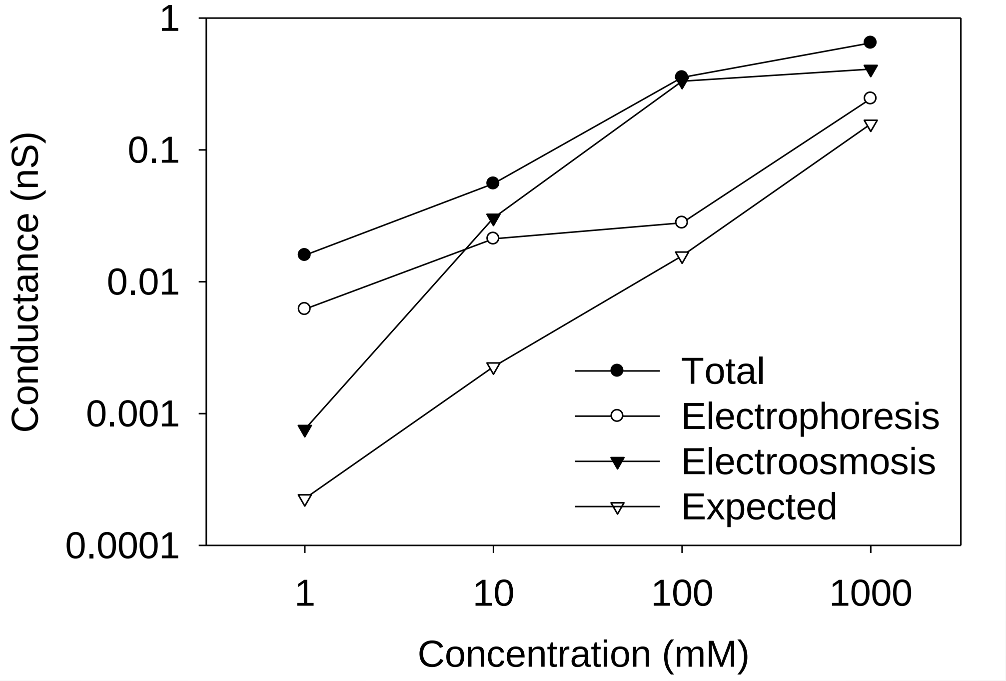
Mesh Convergence

- Triangular mesh elements were used near the mouth of the channel



Results: Conductance

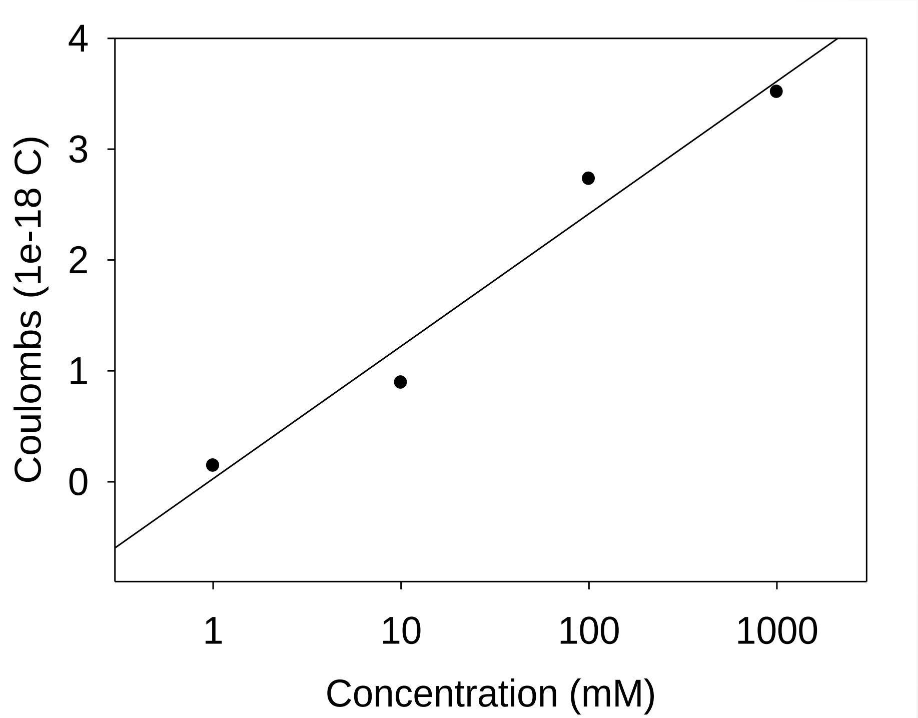
- The conductance/concentration relationship agreed with experimental output
- 2 orders of magnitude increase compared to bulk conductivity theory



Results: Mechanism

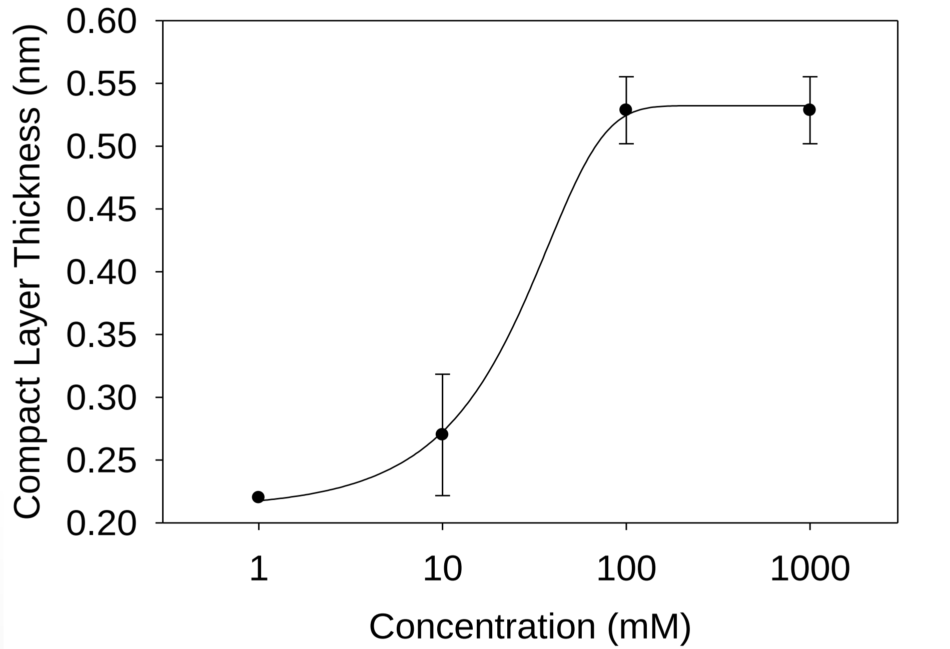
- Electrophoresis at low concentrations
- Electroosmosis at high concentrations
- Net charge increases with concentration

$$\vec{F}_V = F_c \sum^{i} \left(z_j c_j \right) * E$$



Compact Layer Thickness

- Thickness was allowed to vary while the conductance was compared to experimental outputs
- Close to predictions based on assumption of adsorbed molecules



Conclusion

- Demonstrated a stable, rigorous model of electrokinetic flow through SWCNT
- The simulation results agree well with experimental measurements and provide new insight into the unique mechanics of such devices
- Electroosmosis due to increased internal net charge dominates device conductance at higher concentrations
- This study is one of the first to quantitatively define the compact layer thickness

- Acknowledgement
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  - Clemson Palmetto Cluster Super Computing Facility