# Sample Preconcentration in Nanochannels with Nonuniform Surface Charge & Thick Electric Double Layers

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## Introduction

We present an analyte preconcentration method for nanofluidic channels with embedded gate electrodes. The thick electric double layers (EDLs) produced by low concentration electrolytes in our channels can create regions of distinctly different electric fields, leading to nonuniform electromigration fluxes and sample "stacking" near a particular interface.

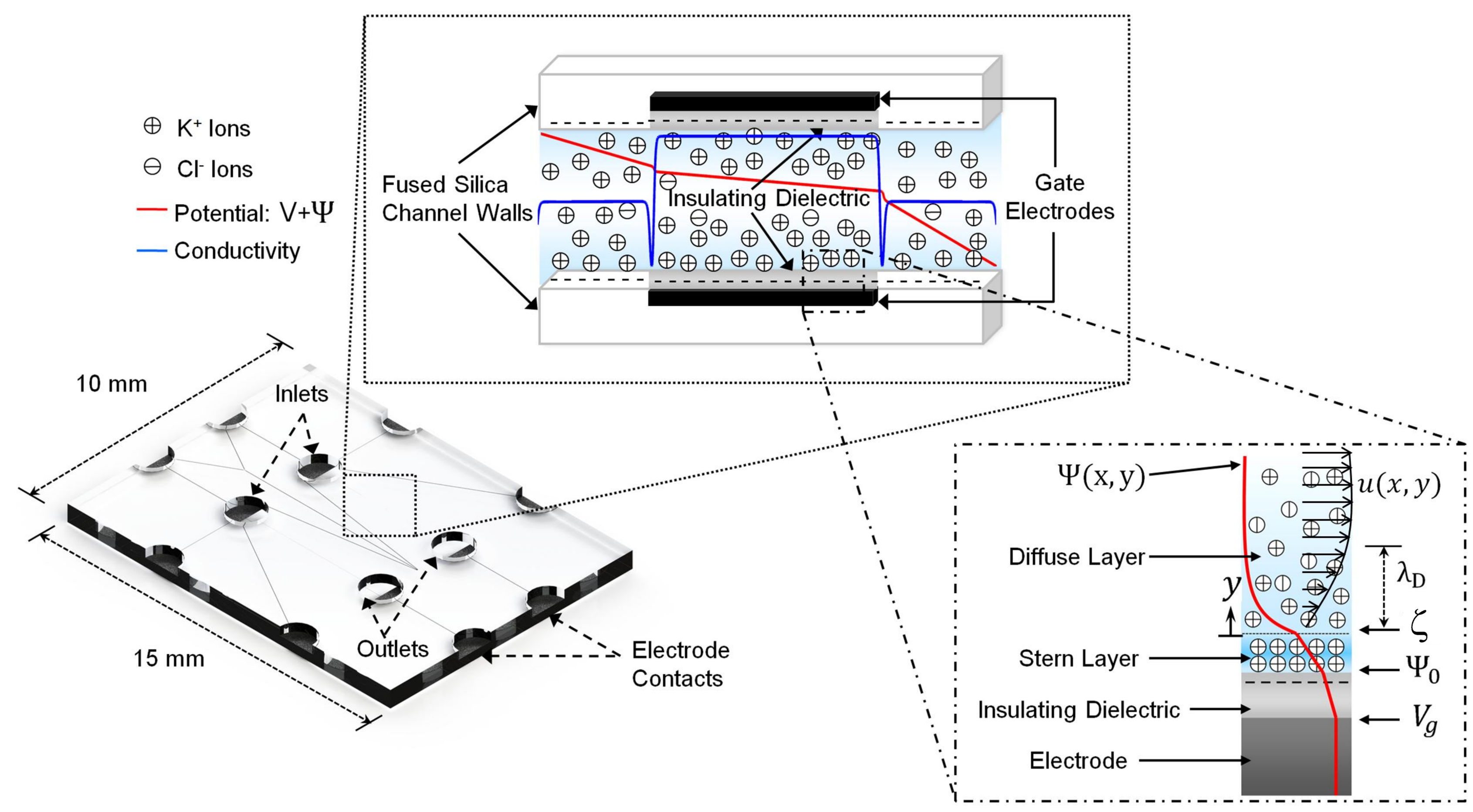


**Figure 1**. Device with embedded electrodes (bottom left). Insets show example ion distributions in the channel (center), as well as the EDL potential and electroosmotic flow (EOF) velocity profile near an embedded electrode (bottom right).

## Computational Methods

- Numerical simulations performed using *COMSOL Multiphysics* v5.1
- Governing equations based on Poisson-Nernst-Planck model
  - EDL potential solved using "*Coefficient Form PDE"* module
  - Electric field solved with "*Electric Currents"* module
  - Velocity field solved using "*Creeping Flow"* module
  - Ionic species conservation solved with "*Transport of Diluted Species"* module

**Poisson's Equation:** $\varepsilon\nabla^2\Psi = -F(c_+ - c_-)$

**Ohm's Law & Current Continuity:** $\mathbf{J} = \sigma_E\mathbf{E}; \quad \mathbf{E} = -\nabla V; \quad \nabla\cdot\mathbf{J} = 0$

**Stokes Equation & Mass Continuity:** $0 = \mu\nabla^2\mathbf{u} - \nabla P + F(c_+ - c_-)\mathbf{E}; \quad \nabla\cdot\mathbf{u} = 0$

**Nernst-Planck Equation:**

$$\frac{\partial c_i}{\partial t} + \mathbf{u}\cdot\nabla c_i = D_i\nabla\cdot\left(\nabla c_i + \frac{e_0 z_i c_i \nabla(V+\Psi)}{k_b T}\right)$$

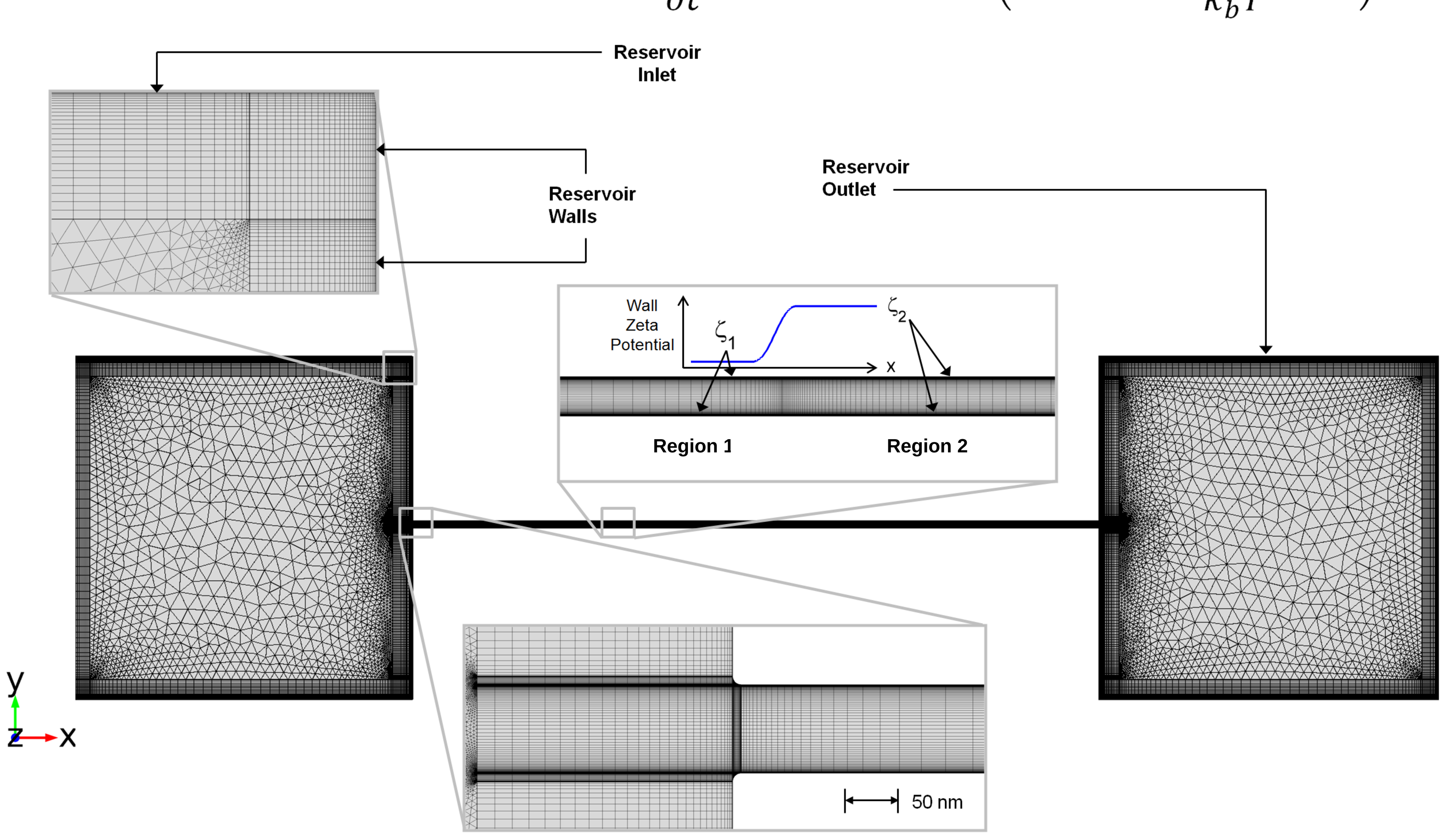


**Figure 2**. COMSOL mesh for the modeled nanochannel and supplying reservoirs.

## Results

Our simulations show considerable sample enhancement for cases with thick electric double layers and large variations in surface potential along the channel, as additional field gradients from thick EDLs cause sample stacking. Resulting profiles compare favorably to analytical models [1-2], and sample enhancement ratios can exceed those from traditional methods[3].

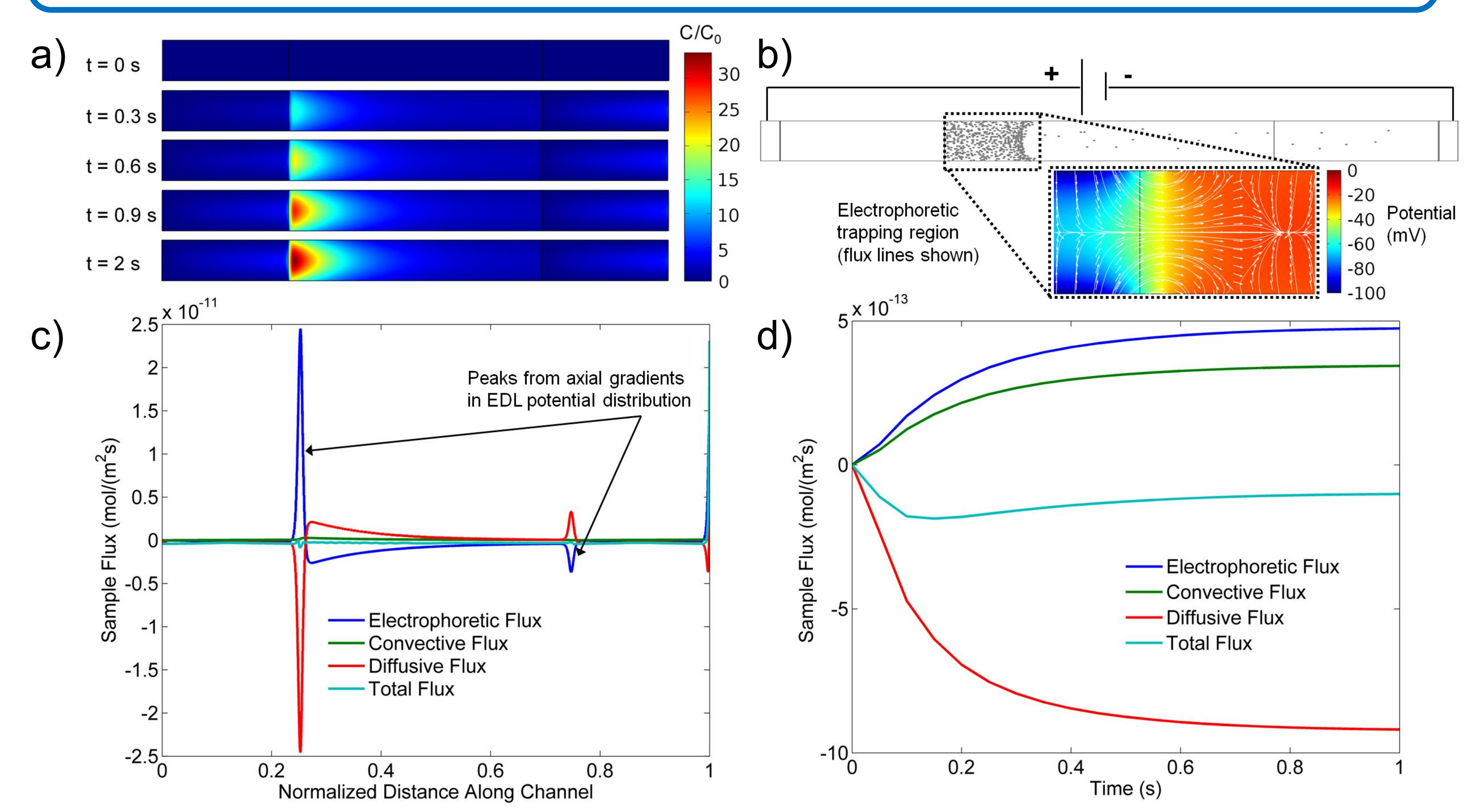


**Figure 3**. (a) Transient 2D sample concentration profiles, (b) electrophoretic particle trapping simulation, (c) steady state fluxes along centerline, and (d) area averaged time-dependent fluxes at the "hot spot".

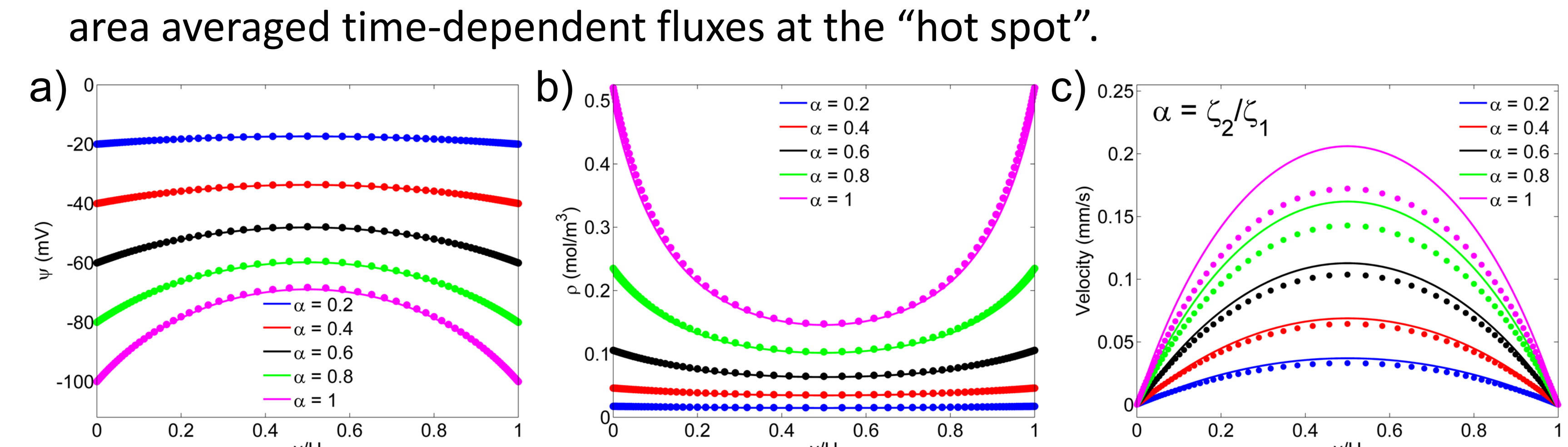


**Figure 4.** Thick EDL profile comparisons: analytical (solid lines) and simulation (solid circles) results for (a) the potential, (b) charge density, and (c) velocity profiles with varying zeta potentials in the middle of the channel.

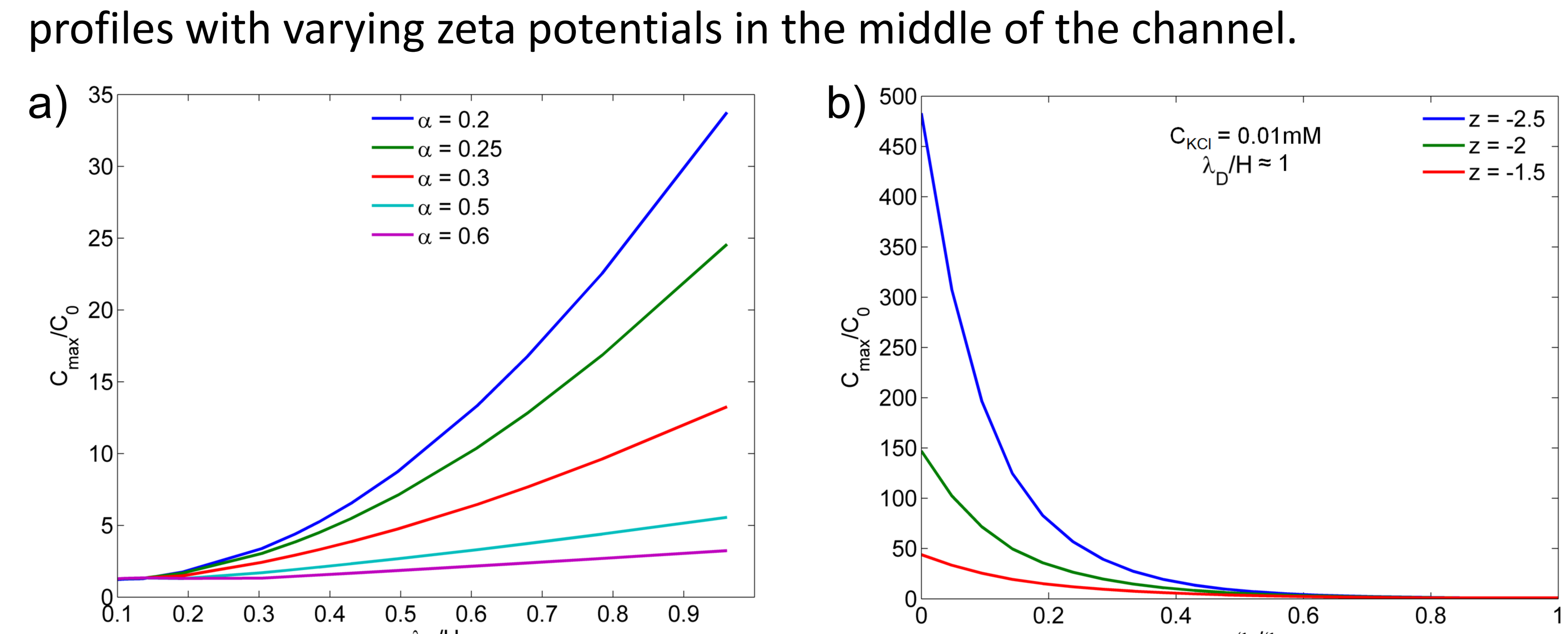


**Figure 5**. (a) Sample enhancement ratios for varying zeta potential & EDL thicknesses, and (b) enhancement for varying zeta potential and sample charge. The zeta potential in region 1 was fixed at -100 mV for these simulations.

## Conclusions

- Axial EDL potential gradients can locally switch direction of net electric field, creating an electrophoretic trapping region
- Method allows for tunable, stationary sample preconcentration in nanochannels without injected plug solution
- Can achieve several hundred-fold sample enhancement
- Less dispersion and greater enhancement than microchannel-based methods[3]

## Acknowledgements

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