Multiphysics Simulation of Ion Concentration Polarization Induced By Nanoporous Membranes in Dual Channel Devices

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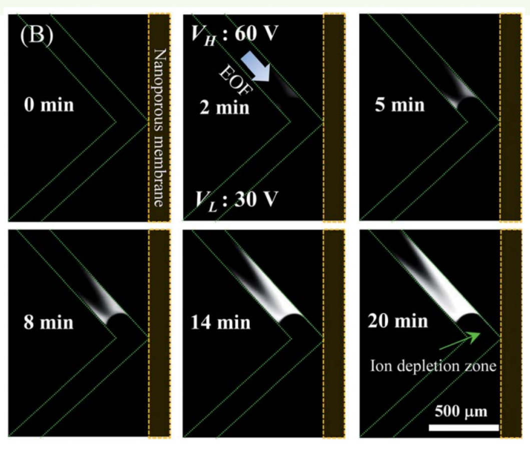
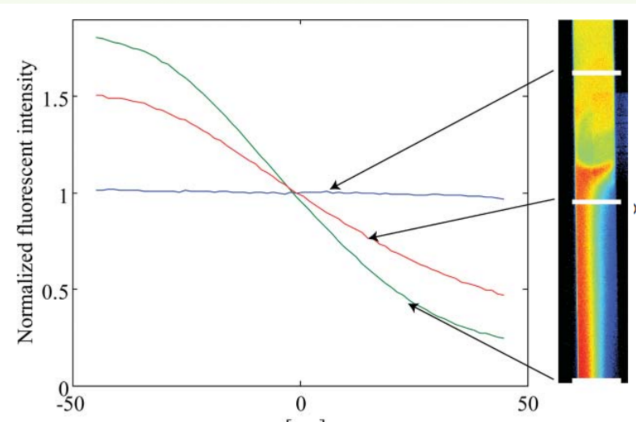
Introduction

Pre-concentration



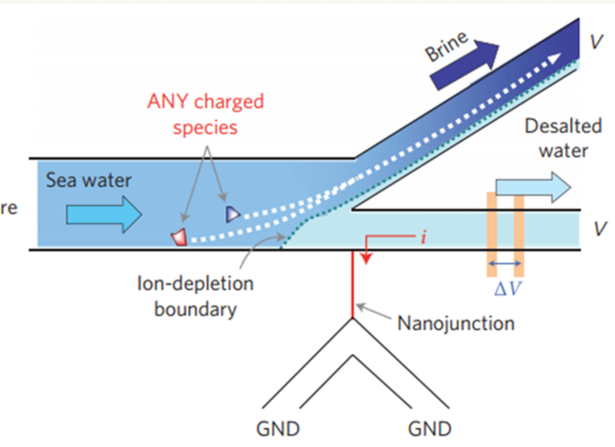
Kim et al., Analyst, 2013. 138(20)

Micromixing



Kim et al., Lab on a Chip, 2008. **8**(4)

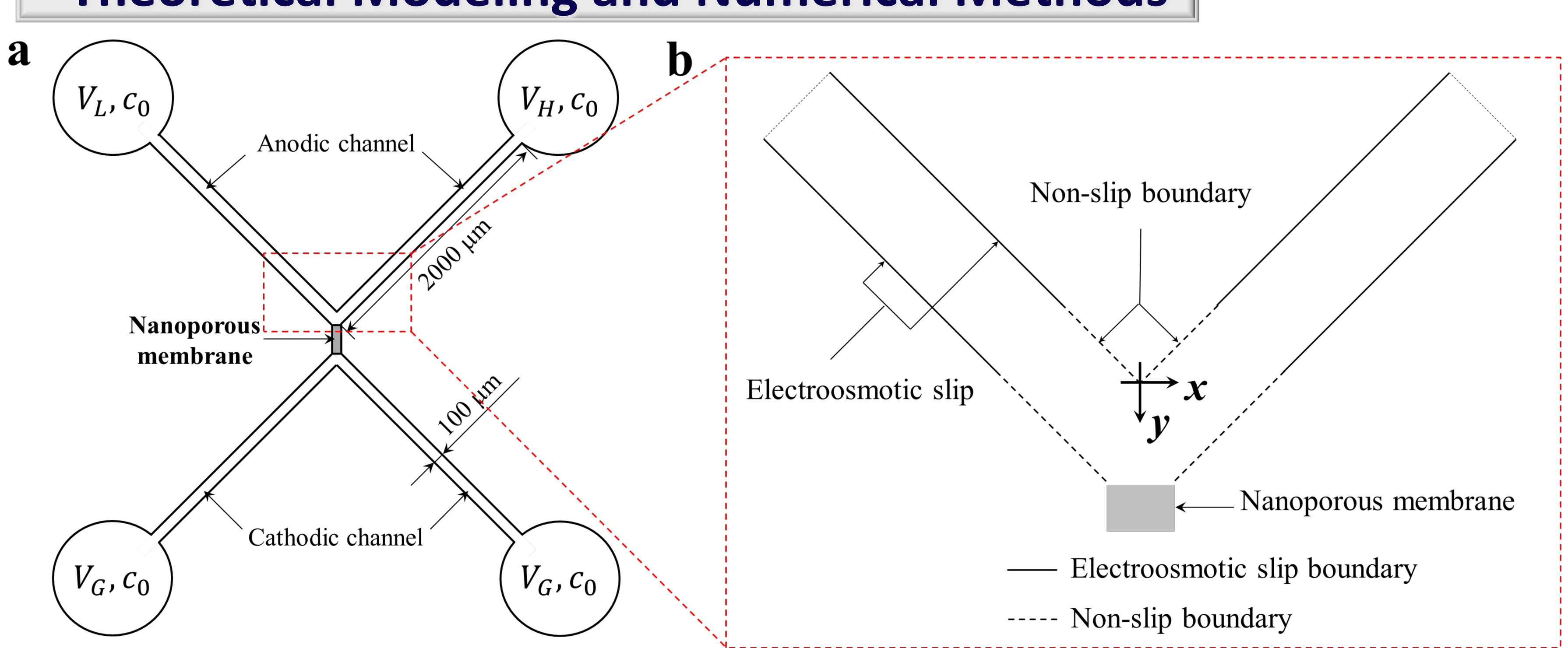
Desalination



Kim et al., Nature Nanotechnology, 2010. 5(4)

- ❖ICP phenomenon has been widely used for fabricating microfluidic devices of pre-concentration, micromixing and desalination.
- ❖However, theoretical research and simulation of ICP have not been carefully dealt with. We provide a multiphysics simulation of a DC-ICP device based on improved numerical settings in this work.

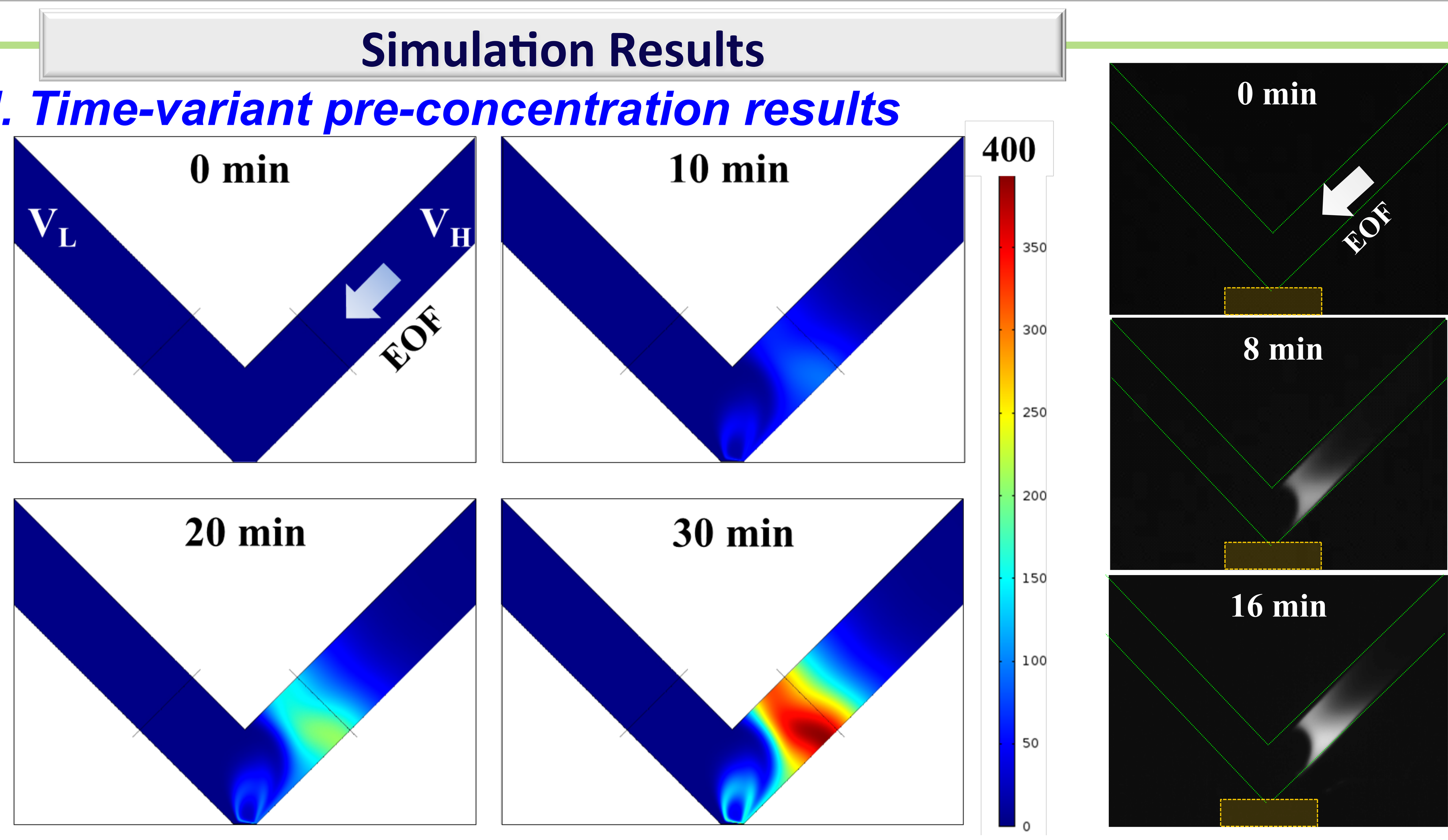
Theoretical Modeling and Numerical Methods



- ❖The modeling was set based on the real experimental conditions as much as possible. Compared to the conventional method, we applied electroosmotic slip boundary condition to connect the slip velocity with the trasient electric field.
- ❖Near the membrane, non-slip boundary condition was applied to release the restriction of electroosmotic slip boundary to vortex flow and its secondary flow.
- ❖The EPM applied in the nanoporous membrane for counter-ions is 4 times large as the value in the bulk solution based on the recent study about the motion of ions and fluid in nanopores.

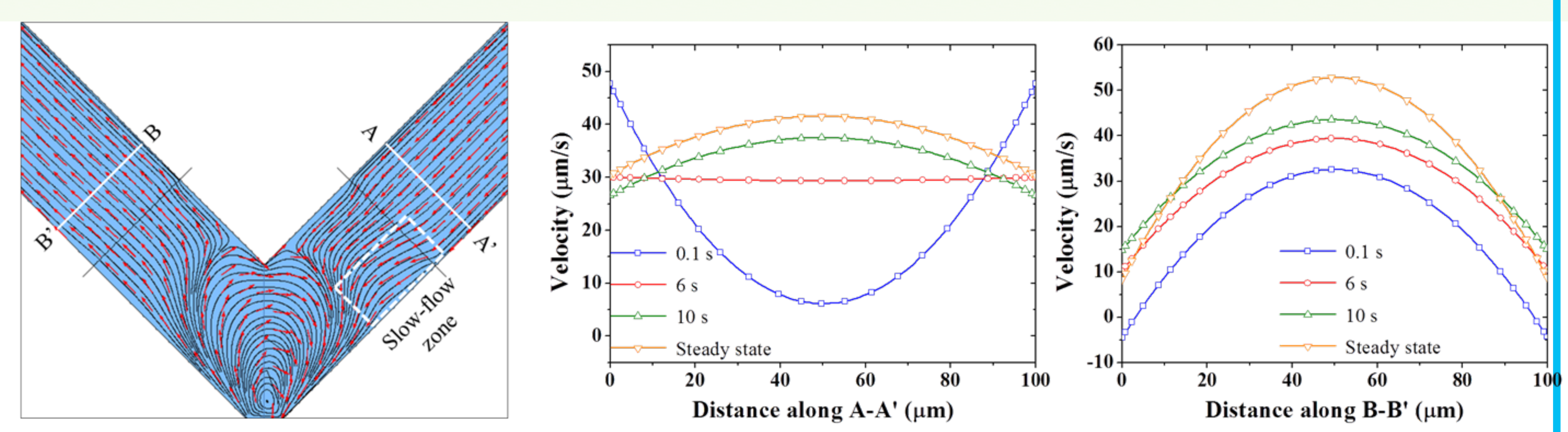
Simulation Results

I. Time-variant pre-concentration results



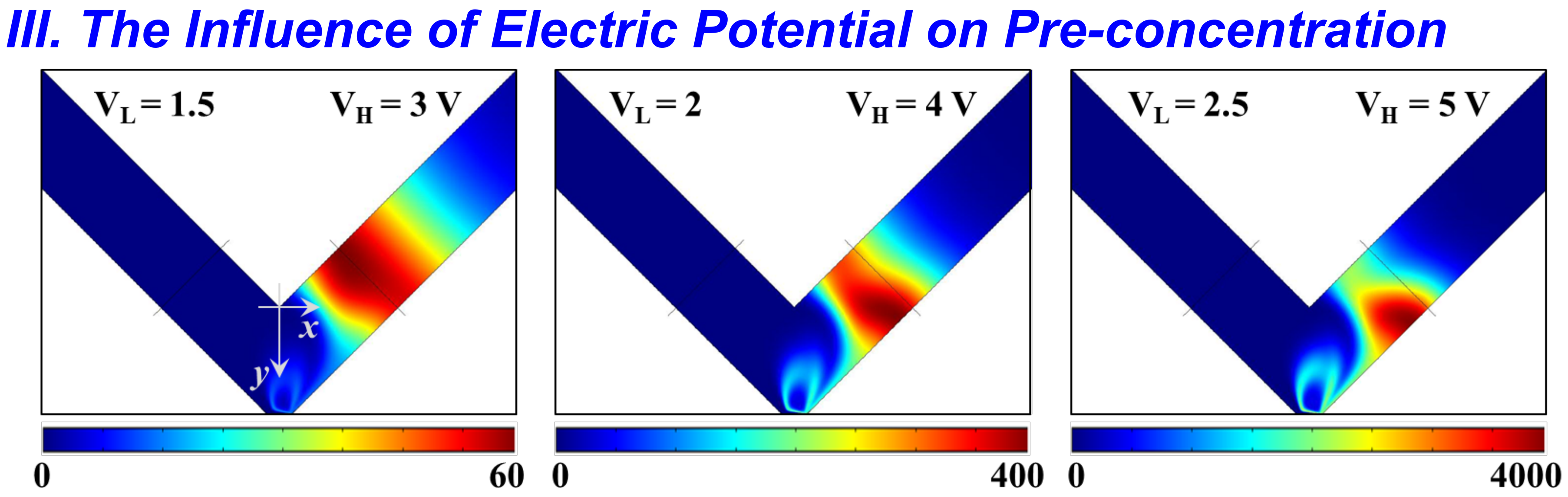
- ❖EOF transports trace molecules from the high voltage end to the low voltage end in the anodic channel. The electrokinetic balance for trace molecules is reached near the ion depletion zone (IDZ) inducing accumulation of trace molecules.
- ❖The qualitative consistency between simulation and experimental results validates our modeling method.
- ❖The ring-shaped concentration of trace molecules near the membrane is caused by the trapping effect of the vortex flow, which is less significant in experiments.

II. Flow Field Distribution Near The Nanoporous Membrane



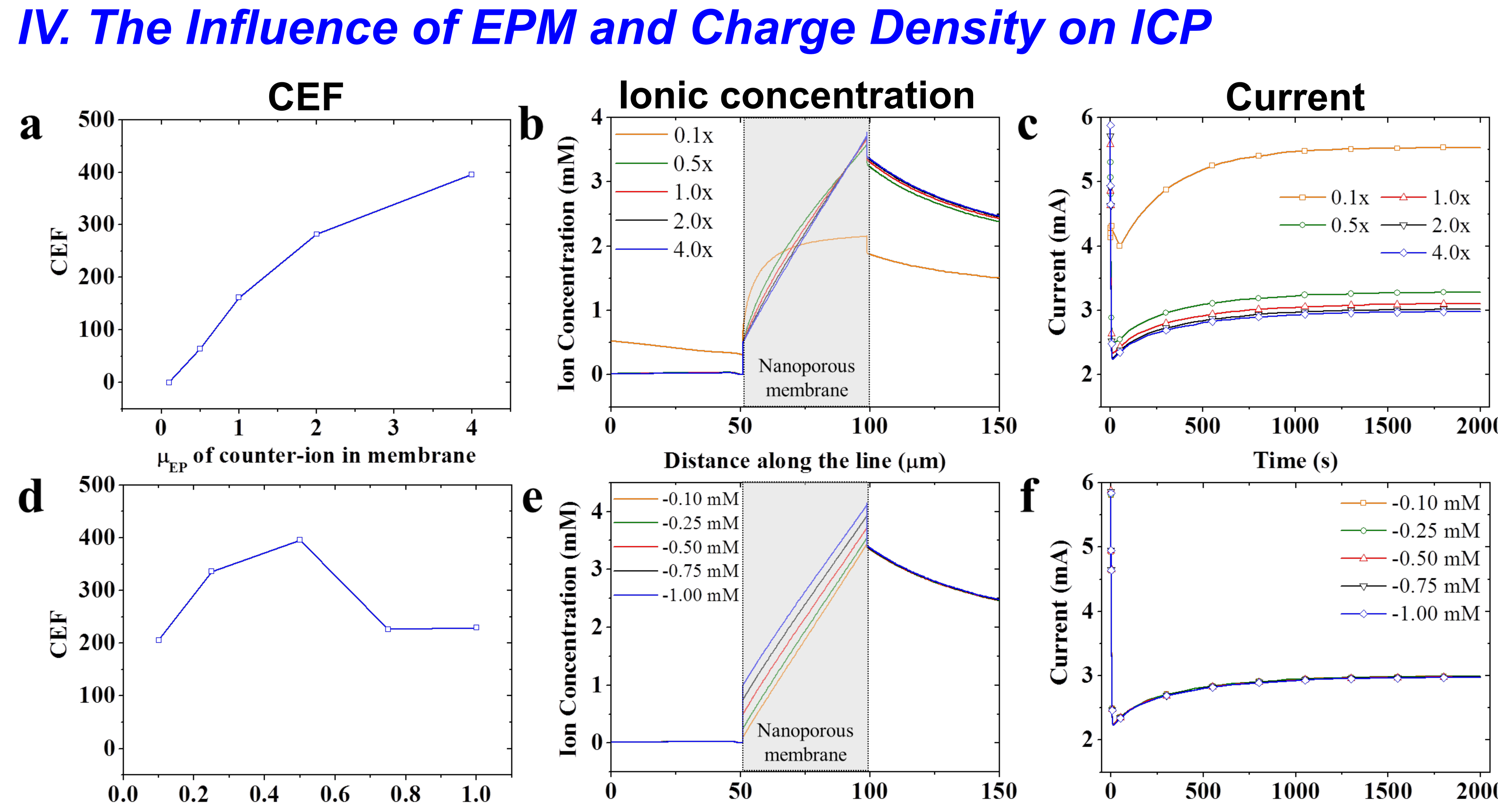
- ❖Vortex flows and secondary flows (slow-flow zone) are generated near the membrane. The velocity of the vortex ranges from 1 mm/s to 20 mm/s which is much faster than the velocity of EOF (~ 40 mm/s).
- ❖The flow velocity at the channel wall is not zero and varies with time because an electroosmotic-slip boundary condition is applied and the electric field along the channel also varies. Consequently, the flow velocity at the channel wall expresses the strength of local electric fields.
- ❖The profile of flow along A-A' or B-B' is not flat as the normal EOF does because the existence of vortex flow enhances the flow rate.

III. The Influence of Electric Potential on Pre-concentration



- ❖The increase of electric potentials can increases the net flux of trace molecules. Additionally, the strength of ICP is enhanced, leading to more effective pre-concentration (higher CEF).
- ❖The profile of concentrated areas gets smaller when the applied electric field is higher because a strong effect of diffusion is made to keep the ion migration balance between electroosmosis and electrophoresis.

IV. The Influence of EPM and Charge Density on ICP



- ❖The results show the influence of different EPMs and charge densities on the results of pre-concentration, ionic concentration distribution across the membrane and current through the channel, respectively.
- ❖It is demonstrated that the EPM of the counter-ions in the membrane plays a more dominant role than the charge density of the membrane in inducing ICP.
- ❖The results reveal that high EPM of counter-ions in the membrane should be applied to obtain good agreement between experiments and simulations
- ❖The shortcomings of traditional simulation methods are significantly improved, in which the EPM of ions in the nanoporous membrane was assumed to be very small because of local low permeability that neglects the flow inside the membrane.

Conclusions

1. We have simulated ICP development and vortex generation in a DC-ICP device with improved boundary conditions and a wide range of EPMs of counter-ions and charge densities in a nanoporous membrane.
2. We validated the 2-D model and simulation results with experimental ones in terms of CEFs, ion concentrations, electric fields (ionic currents), and flow fields under various electric potentials.
3. It was demonstrated that pre-concentration is significantly affected by electric potentials and flow fields including vortex flows and a slow-flow zone induced near the nanoporous membrane.
4. We found that the EPMs of counter-ions in the nanoporous membrane play key roles in ICP phenomena.

References

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