Mathematical Modeling of Electrokinetic Micropumps

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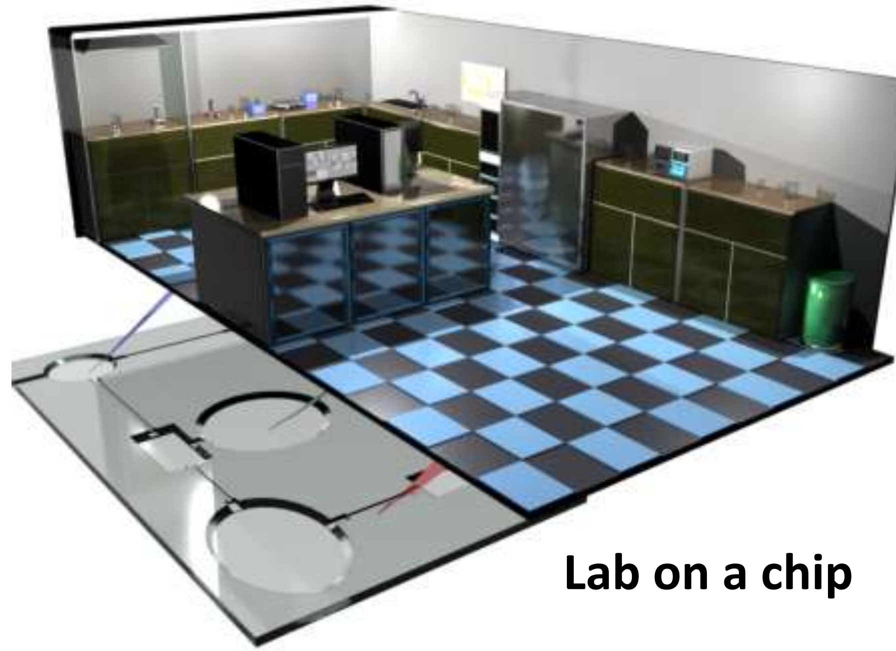
INSTITUTE OF CHEMICAL TECHNOLOGY PRAGUE

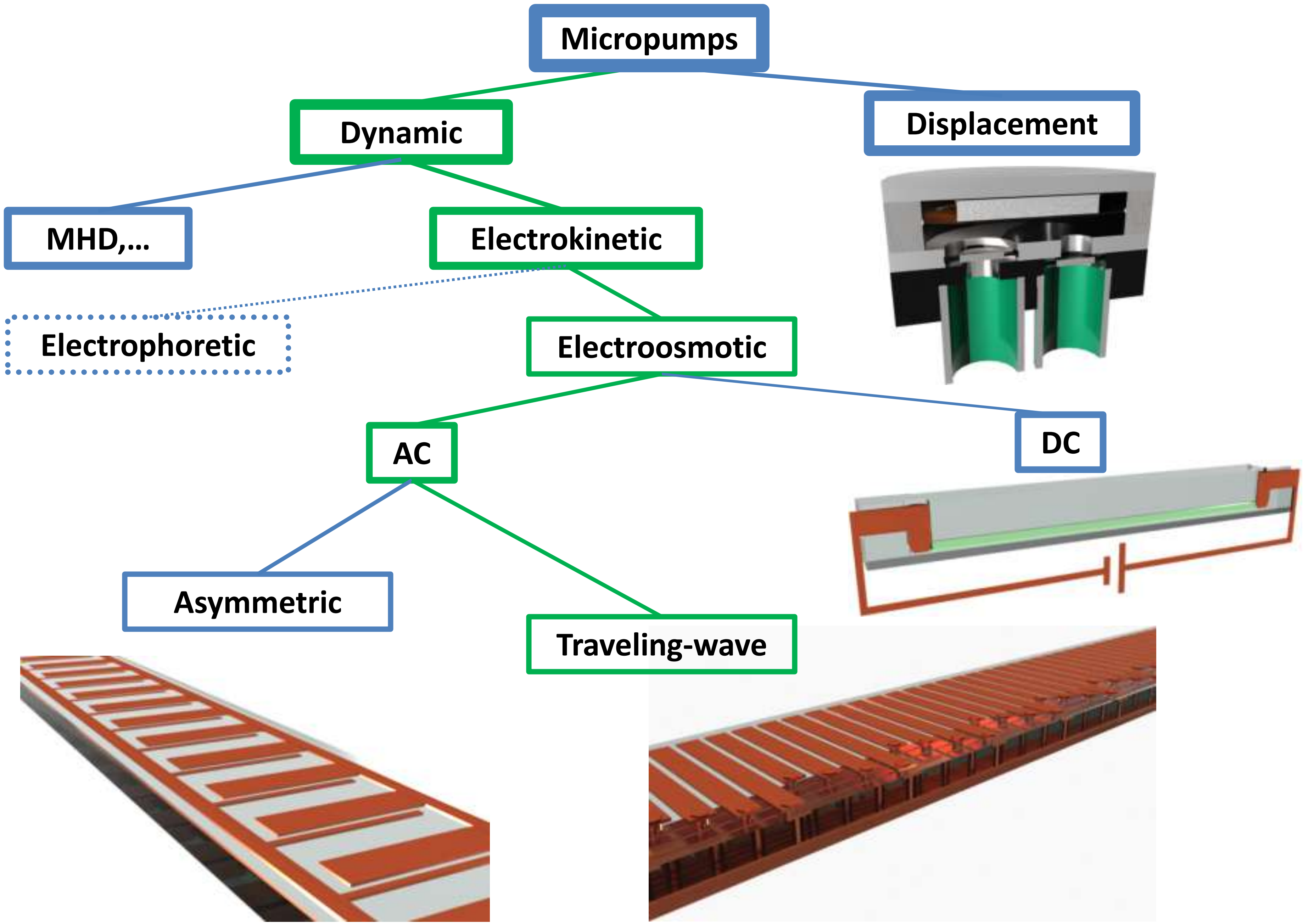


Lab on a chip

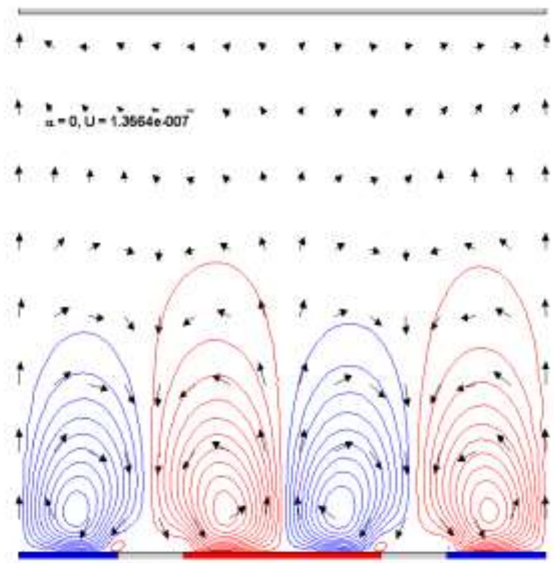
Outline

- **Pumping in micro- and nanoscale**
- **Interfacial phenomena and Electroosmotic flow**
- **Mathematical model equations**
- **Software implementation**
  - Model geometry and boundary conditions
  - Spatial discretisation and model solution
- **Results discussion**
  - Model quantities profiles
  - Velocity characteristics
- **Conclusions**

Pumping in micro- and nanoscale



Pumping in micro- and nanoscale

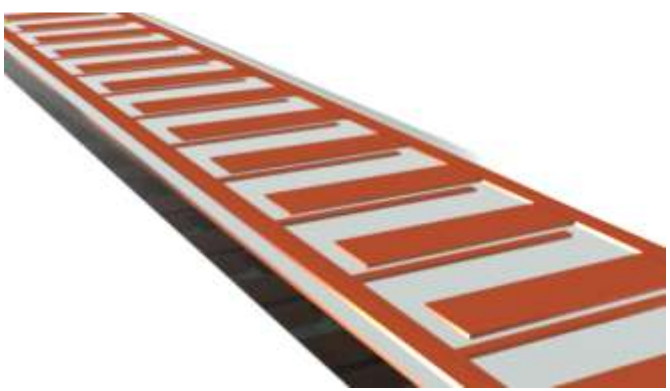


- Symmetrical designs produce no net flow

AC electro-osmotic

Asymmetric

Traveling-wave



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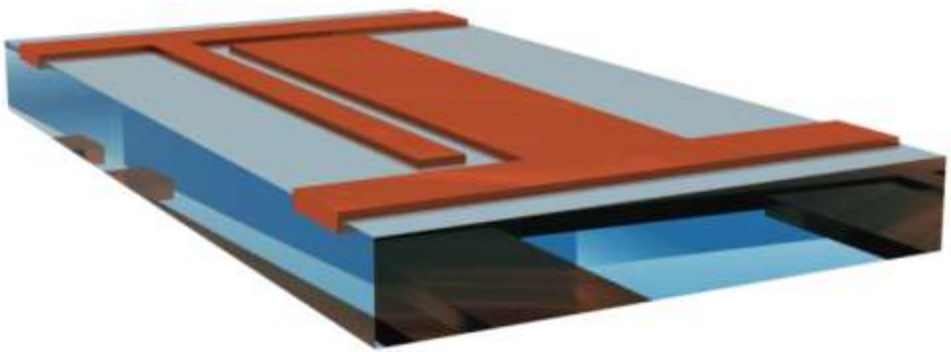

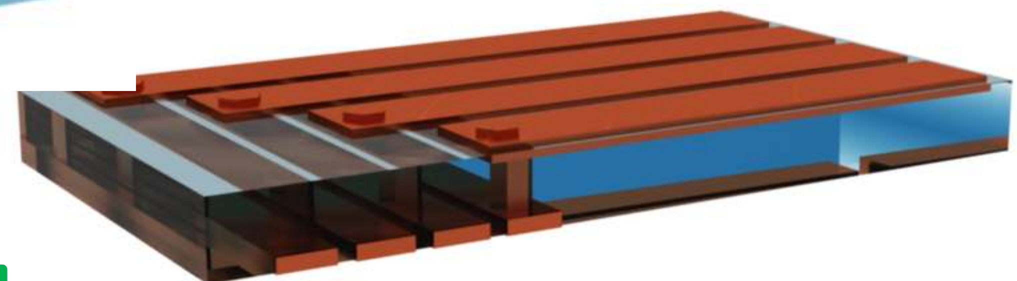

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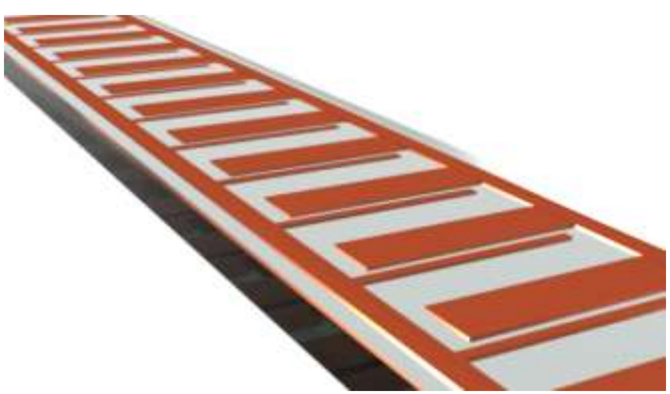
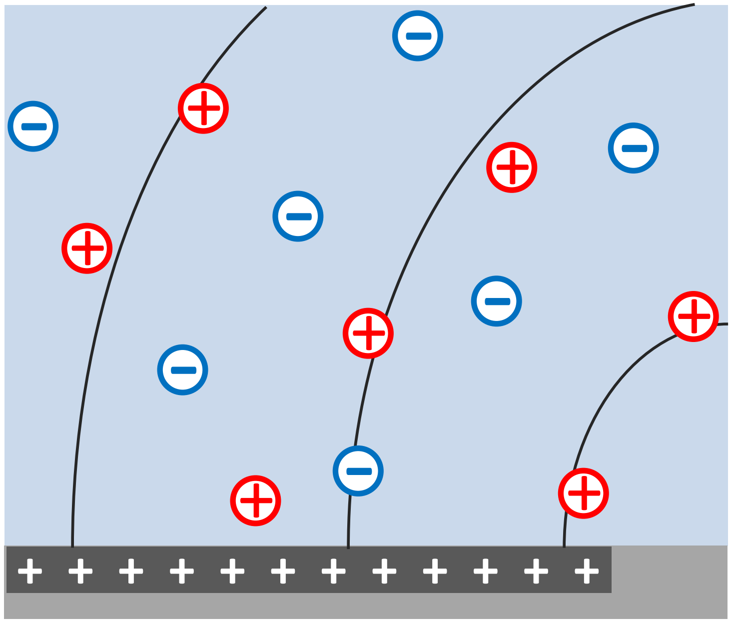


Interfacial phenomena and Electroosmotic flow

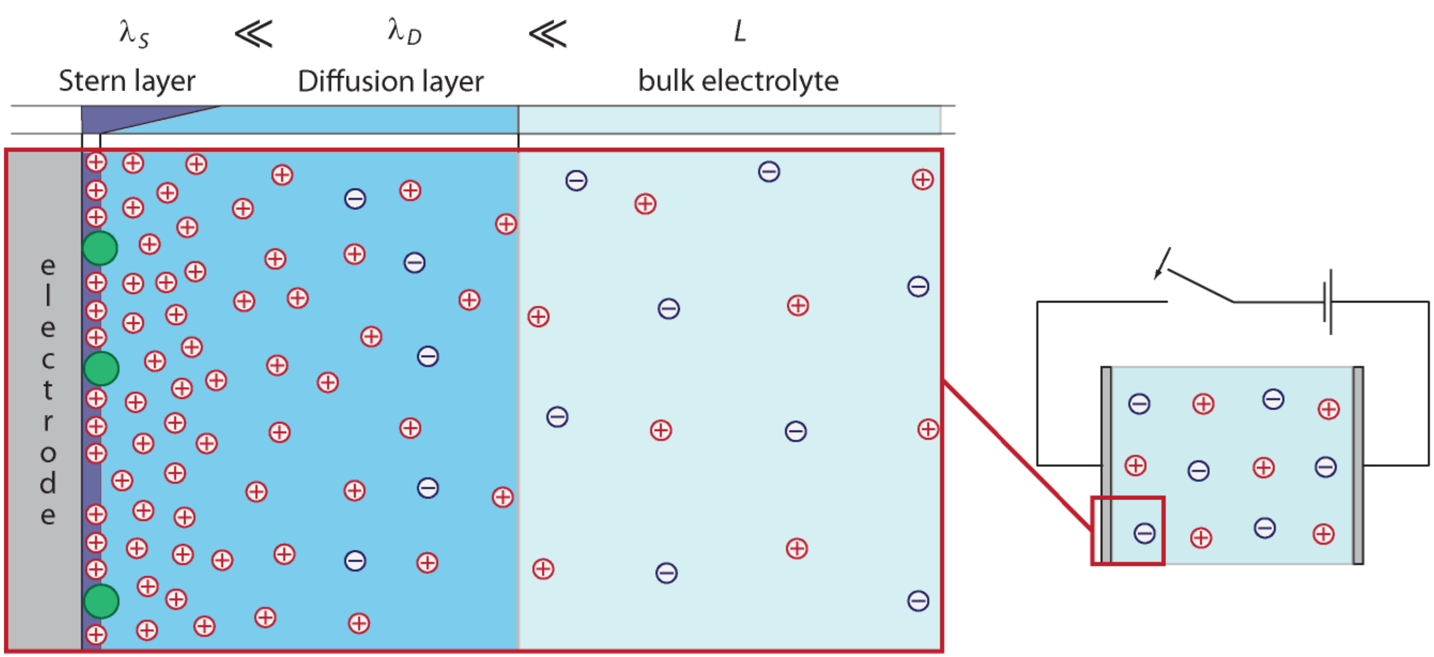


Normal component of the electric intensity vector

- Ions are attracted or repeled by the Coulombic force

$$f_e^{\perp} = qE^{\perp} = -q\frac{\partial \varphi}{\partial y}$$

- Ion concentrations change exponentialy toward the charged wall.
- Coulombic force compete with diffusion
- There is non-zero charge density in electric double-layer, shielding



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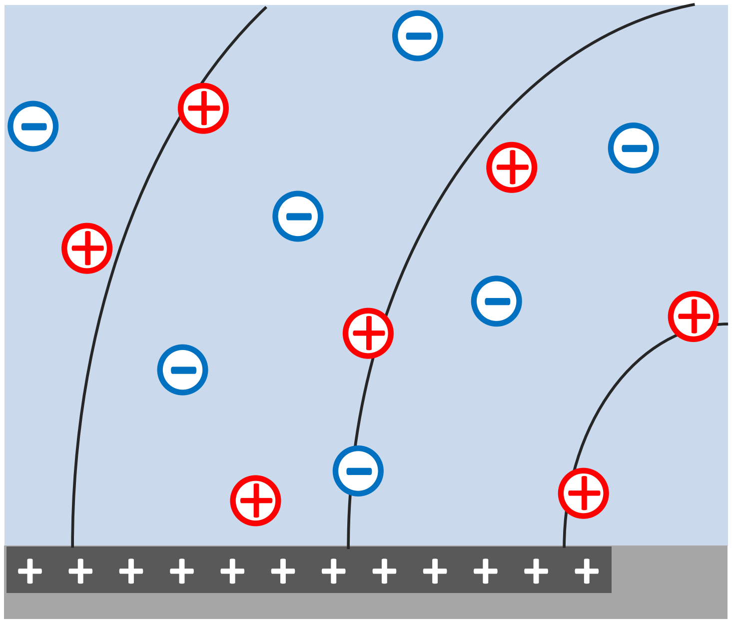

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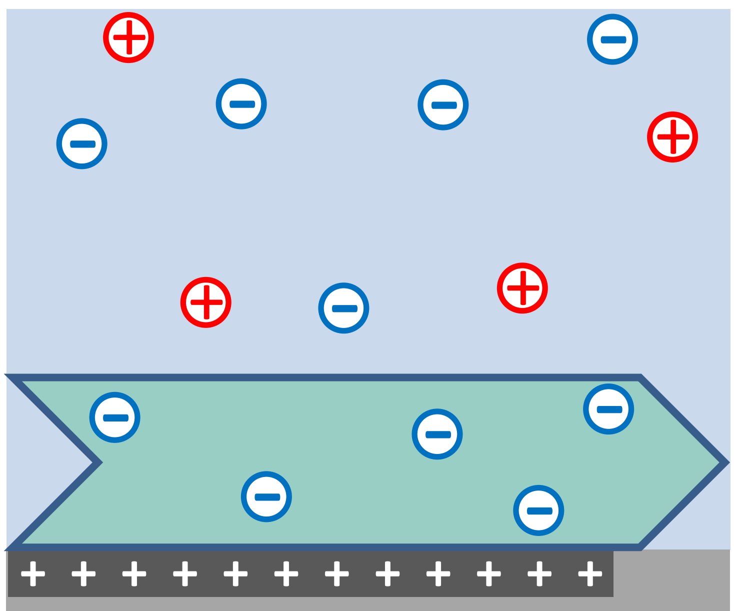

Tangential component of the electric intensity vector

- Accumulated ions are dragged by Coulombic force along the surface

$$f_e^{||} = qE^{||} = -q\frac{\partial \varphi}{\partial x}$$

- Momentum is transported into the electrolyte bulk via viscous forces

$$\mathbf{f}_\eta = -\nabla \cdot (-\eta \nabla \mathbf{v}) = \eta \nabla^2 \mathbf{v}$$

Mathematical model equations

Full model

Electrochemical problem

Poisson equation

$$0 = -\tilde{\boldsymbol{\nabla}} \cdot (\tilde{\boldsymbol{\nabla}} \tilde{\varphi}) - \frac{\tilde{q}}{\tilde{\lambda}_D^2}$$

Local mass balances

$$\frac{1}{\tilde{\lambda}_D} \frac{\partial \tilde{c}}{\partial \tilde{t}} = -\tilde{\boldsymbol{\nabla}} \cdot \left[\tilde{\mathbf{v}} \tilde{c} - \tilde{\boldsymbol{\nabla}} \tilde{c} - \tilde{q} \tilde{\boldsymbol{\nabla}} \tilde{\varphi} \right]$$

$$\frac{1}{\tilde{\lambda}_D} \frac{\partial \tilde{q}}{\partial \tilde{t}} = -\tilde{\boldsymbol{\nabla}} \cdot \left[\tilde{\mathbf{v}} \tilde{q} - \tilde{\boldsymbol{\nabla}} \tilde{q} - \tilde{q} \tilde{\boldsymbol{\nabla}} \tilde{\varphi} \right] - \frac{\tilde{q}}{\tilde{\lambda}_D^2}$$

Hydromechanical problem

Navier-Stokes equation

$$\frac{1}{\tilde{\lambda}_D} \frac{1}{\mathrm{Sc}} \frac{\partial \tilde{\mathbf{v}}}{\partial \tilde{t}} = -\tilde{\boldsymbol{\nabla}} \tilde{p} - \tilde{\boldsymbol{\nabla}} \cdot \left(\frac{\tilde{\mathbf{v}} \tilde{\mathbf{v}}}{\mathrm{Sc}} - \tilde{\boldsymbol{\nabla}} \tilde{\mathbf{v}} \right) - \frac{\mathrm{Ra}}{\tilde{\lambda}_D^2} \tilde{q} \tilde{\boldsymbol{\nabla}} \tilde{\varphi}$$

Continuity equation

$$0 = \tilde{\boldsymbol{\nabla}} \cdot \tilde{\mathbf{v}}$$

$$\tilde{\mathbf{x}} = (\tilde{x}, \tilde{y}) = (x/L, y/L), \ \tilde{t} = \frac{t}{t_\circ}$$

$$\nabla_\circ = \frac{1}{L}, \ \varphi_\circ = \frac{RT}{F}, \ q_\circ = 2 c_\circ F, \ t_\circ = \frac{\lambda_D}{v_\circ}, \ v_\circ = \frac{D}{L}, \ p_\circ = \frac{v_\circ \eta_\circ}{L}$$

$$\tilde{\varphi} = \frac{\varphi}{\varphi_\circ}, \ \tilde{c} = \frac{c^+ + c^-}{2 c_\circ} - 1, \ \tilde{q} = \frac{c^+ - c^-}{2 c_\circ}, \ \tilde{\mathbf{v}} = \frac{\mathbf{v}}{v_\circ}, \ \tilde{p} = \frac{p}{p_\circ}$$

Mathematical model equations

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Navier-Stokes equation

$$0 = \tilde{\boldsymbol{\nabla}} \cdot \tilde{\mathbf{v}}$$

Continuity equation

Linearized model

$$\tilde{\boldsymbol{\nabla}}^2 \tilde{\psi} = 0, \quad \tilde{\boldsymbol{\nabla}}^2 \hat{\tilde{\mathbf{v}}} = \tilde{\boldsymbol{\nabla}} \hat{\tilde{p}}, \quad \tilde{\boldsymbol{\nabla}} \cdot \hat{\tilde{\mathbf{v}}} = 0$$

Laplace and Stokes equation

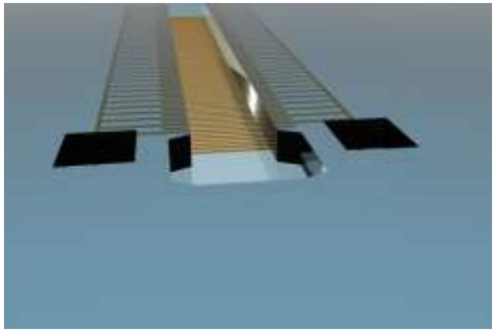
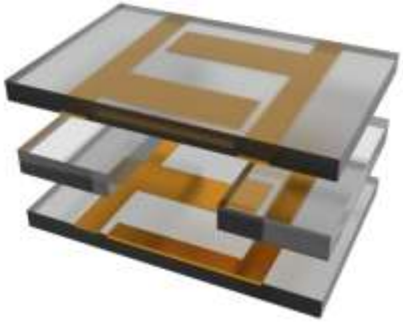
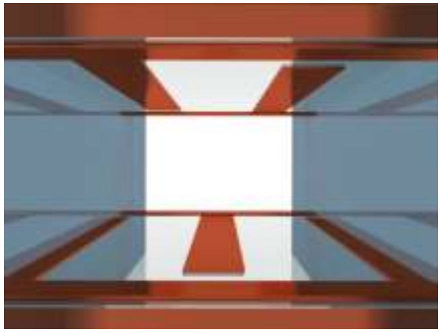
$$\frac{\partial \tilde{\psi}}{\partial \tilde{y}} = +i \left(\tilde{\psi} - \tilde{\psi}_m \right), \quad \frac{\partial \tilde{\psi}}{\partial \tilde{y}} = -i \left(\tilde{\psi} - \tilde{\psi}_m \right), \quad \frac{\partial \tilde{\psi}}{\partial \tilde{y}} = 0$$

RC boundary conditions

$$\frac{\hat{\tilde{u}}}{\mathrm{Ra}} = \frac{1}{2} \Re \left[\left(\tilde{\psi} - \tilde{\psi}_m \right) \frac{\partial \tilde{\psi}^*}{\partial \tilde{x}} \right]$$

Helmholtz-Smoluchowski equation

Model geometry and boundary conditions

An assumption of the system-properties periodicity implies the periodicity in electrode array

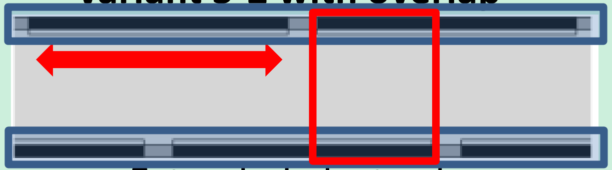
variant 5-0

Bottom arrangement

variant 3-2

Shift of even electrodes

variant 3-2 with overlap



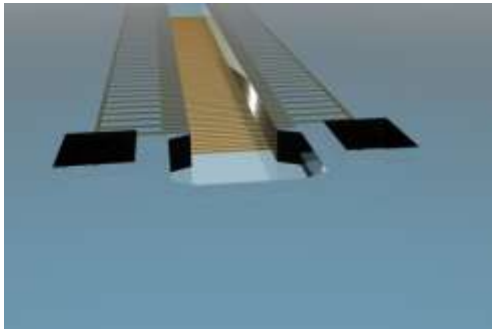
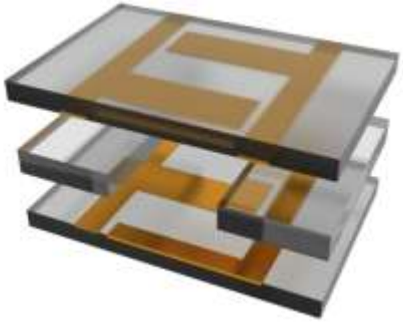
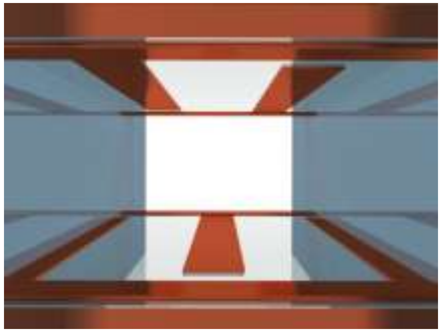
Extended electrodes

Electrode overlap brings new quality to model behavior

The boundary conditions and initial approximation

- Four-phase arrays require more than one coustruction layer (x spiral design)
- The more surface is covered by electrodes, the stronger is fluid flow
- Flow reversal seems to be generic feature of zig-zag arrangement

Model geometry and boundary conditions

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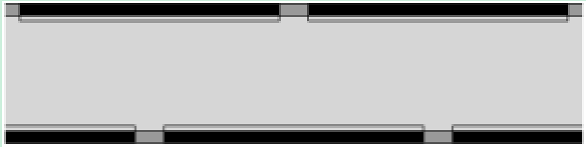

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The boundary conditions and initial approximation

Electrode surfaces

$$\varphi_i = A \sin\left(\omega t + i\frac{2\pi}{n}\right), \quad i = 0, 1, 2, 3$$

Solid-electrolyte interface

$$\mathbf{n}\cdot\mathbf{J}^{\pm} = 0, \quad \mathbf{n}\cdot\nabla\varphi = 0, \quad \mathbf{v} = (0, 0)$$

Left and right margin (periodicity)

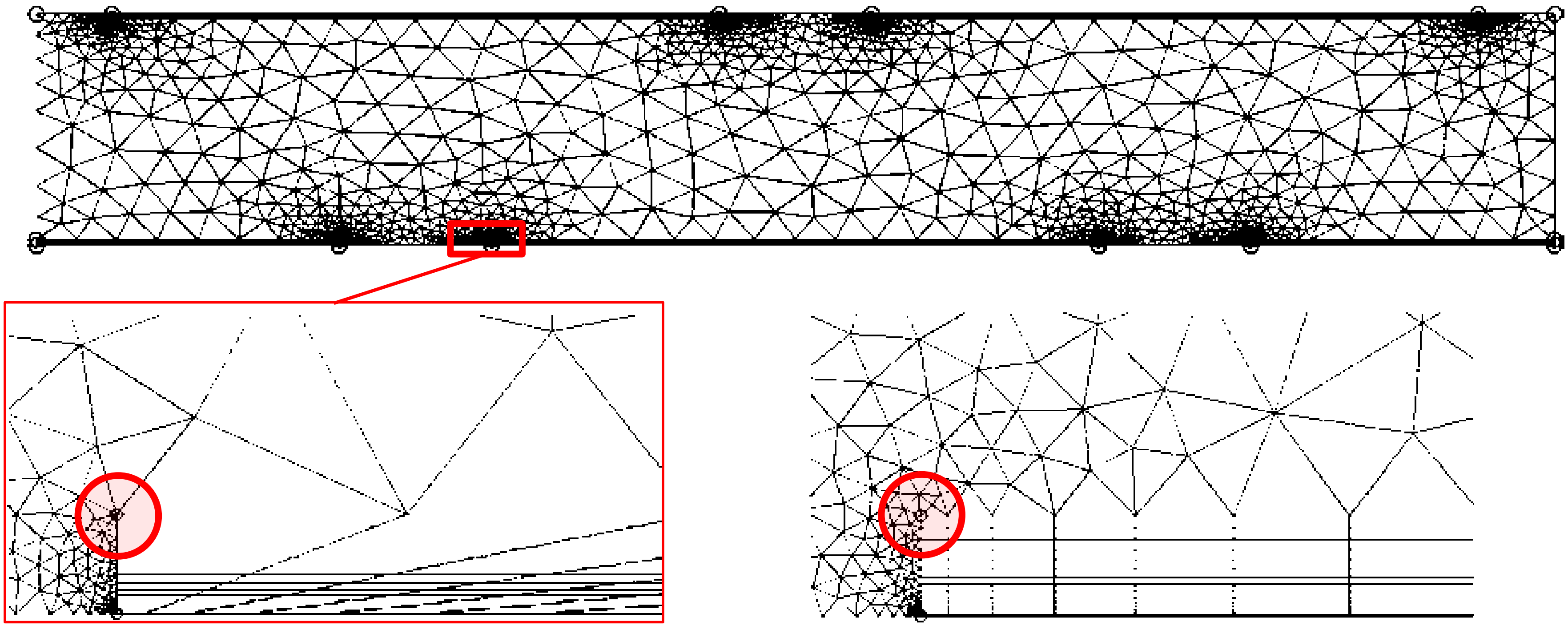
$$\xi(x, y, t) = \xi(x + L, y, t)$$
$$\xi = \{\varphi, c^{\pm}, \mathbf{v}, p\}$$

Initial approximation

$$\varphi(0, x, y) = 0, \quad c^{+}(0, x, y) = c^{-}(0, x, y) = c_0$$

Spatial discretization and model solution

Hybrid discretization mesh

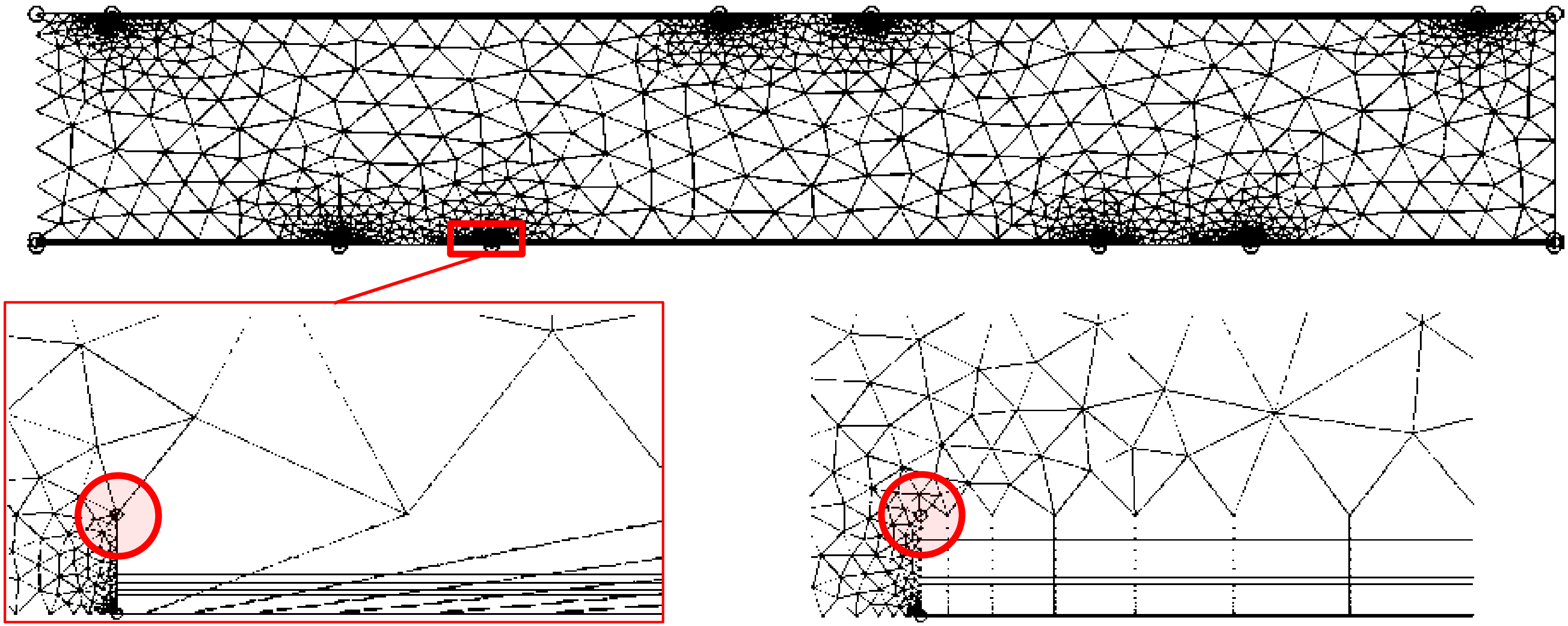


An advantage of skewed quadrilateral mesh

- Supress element densification above the electrode corners

Spatial discretization and model solution

Hybrid discretization mesh

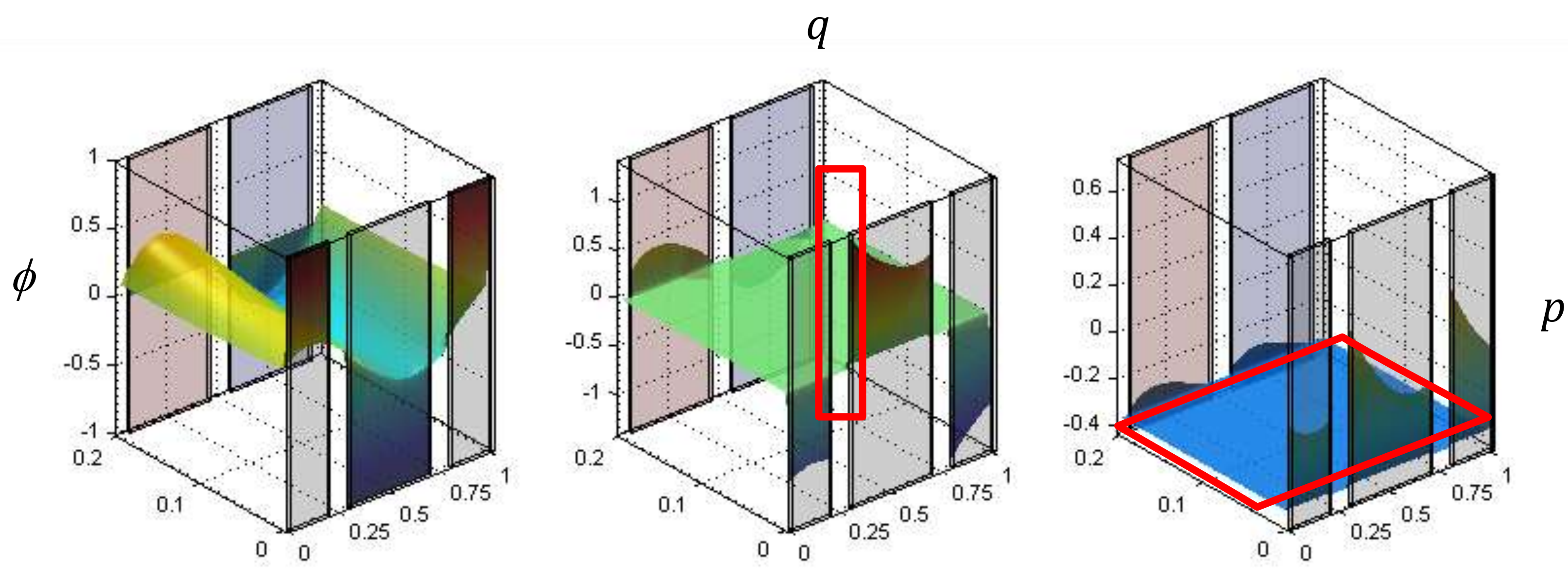


Used mathematical method and solver

- **Software:** Matlab 2007a & COMSOL Multiphysics 3.4a
- **Method:** FEM
- **FE type:** Lagrange, 2nd order, triangular and (skewed) quadrilateral
- **FE count range:** 2500-16000, **Typical FE count:** 4000-5000
- **Solver:** femtime (pardiso, UMFpack)

Profiles of model quantities

- The spatio-temporal profiles of the electric potential, the electric charge density and the pressure

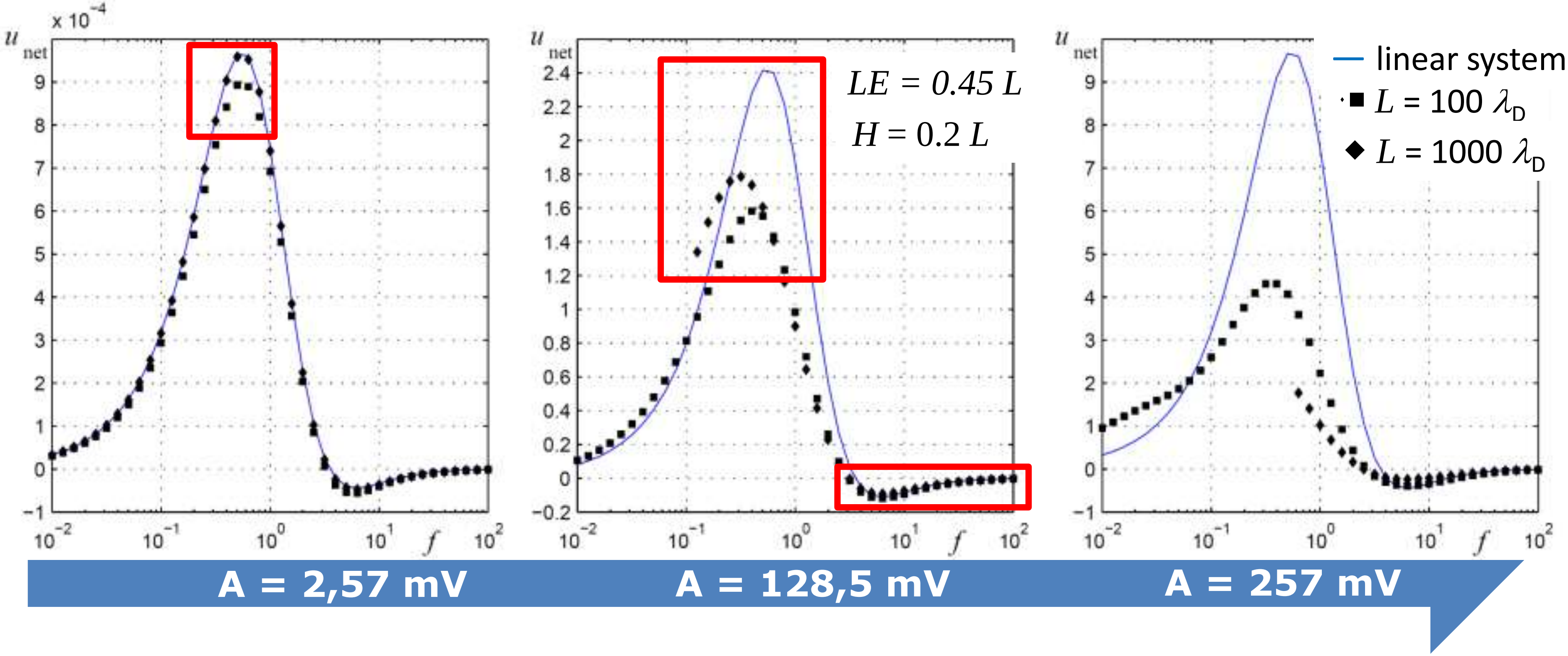


- The largest gradients of the physical fields occur near to the electrode corners

- The changes in physical quantities are restricted to the narrow zones close to the electrode surfaces

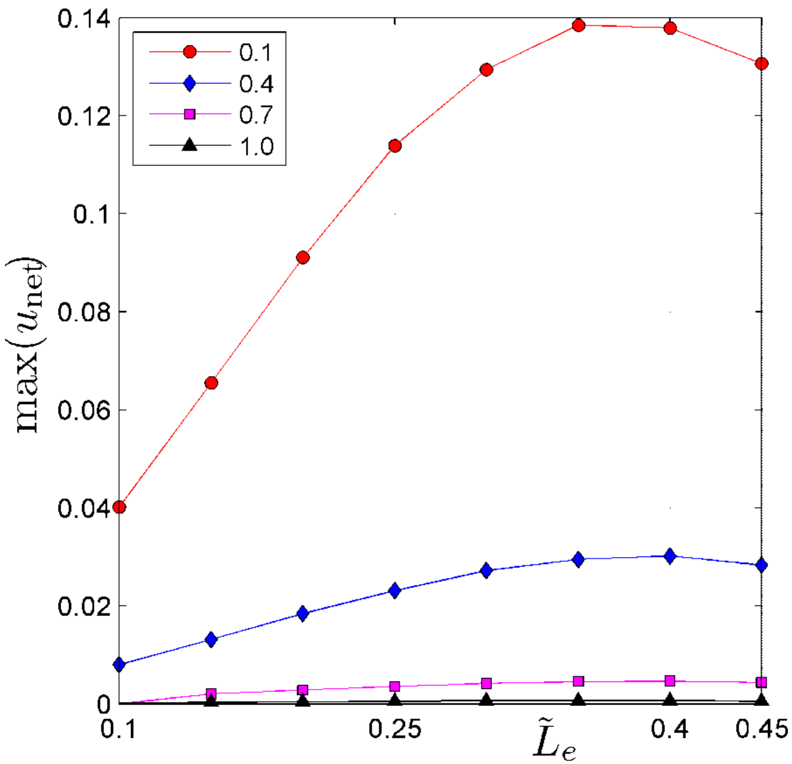
Net velocity characteristics

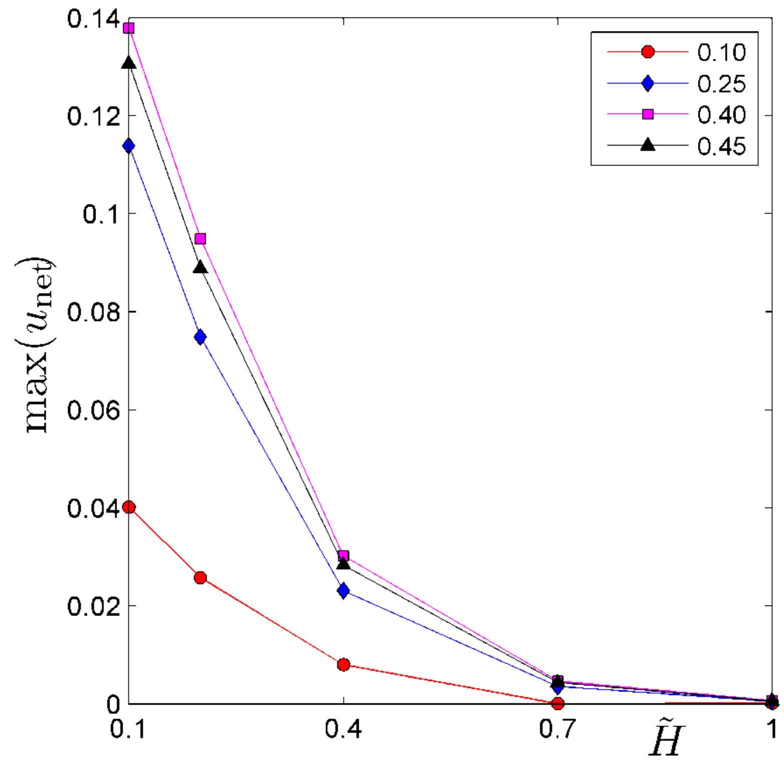
$$u_{\rm net} = \frac{1}{T}\frac{1}{LH}\int_{t}^{t+T}\left(\iint_{\tilde{\mathcal{D}}} \tilde{u}(\tilde{\mathbf{x}},\tilde{t})\,\mathrm{d}\tilde{\mathbf{x}}\right)\mathrm{d}\tilde{t}, \quad \tilde{\mathcal{D}} = [0,1)\times[0,\tilde{H}], \quad \tilde{t}\in[11,12]T_\circ, \quad u_\circ = \frac{D}{L}, \quad t_\circ = \frac{\lambda_D L}{D}$$



- There are discrepancies between data obtained by the linear and nonlinear models.
- With increased voltage, optimal frequencies drop to lower values.
- At higher frquencies, the direction of fluid flow changes, the flow reversal occurs.

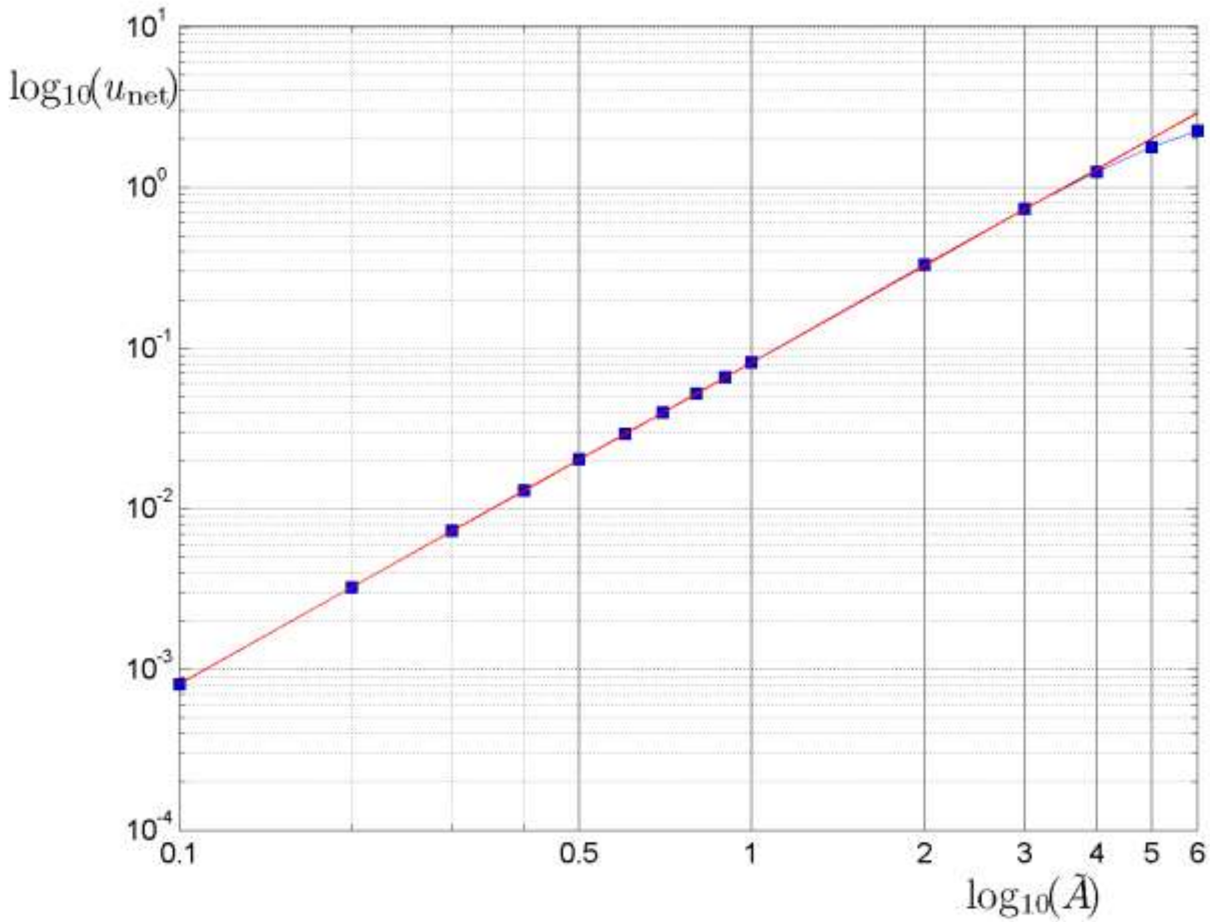
Net velocity characteristics – geometric parameters





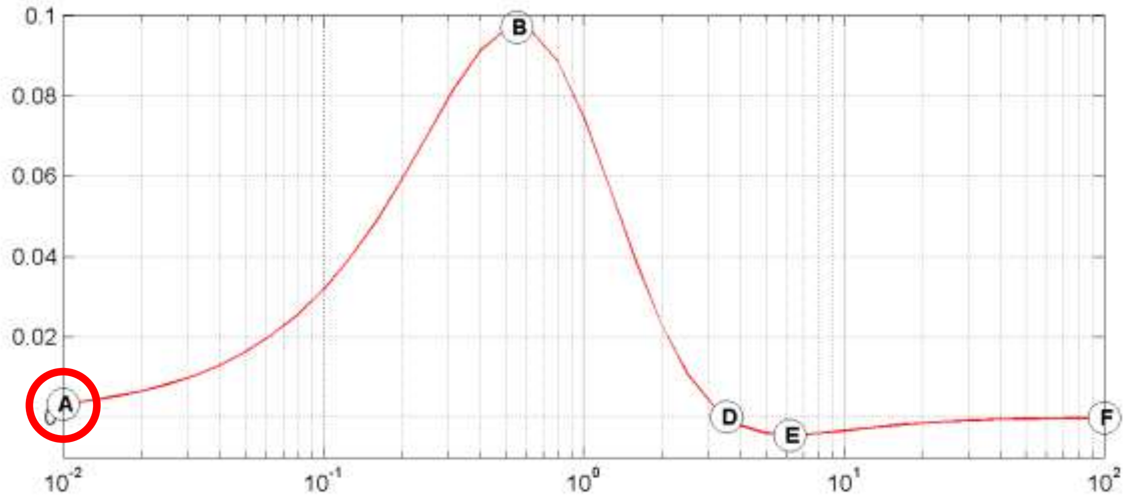
- There is an optimal electrode width, 30-40 % L
- The net velocity decrease rapidly with the increasing channel height

Net velocity characteristics – voltage



- The net velocity is proportional to square of the voltage
- At higher voltages, the velocity increase slows down

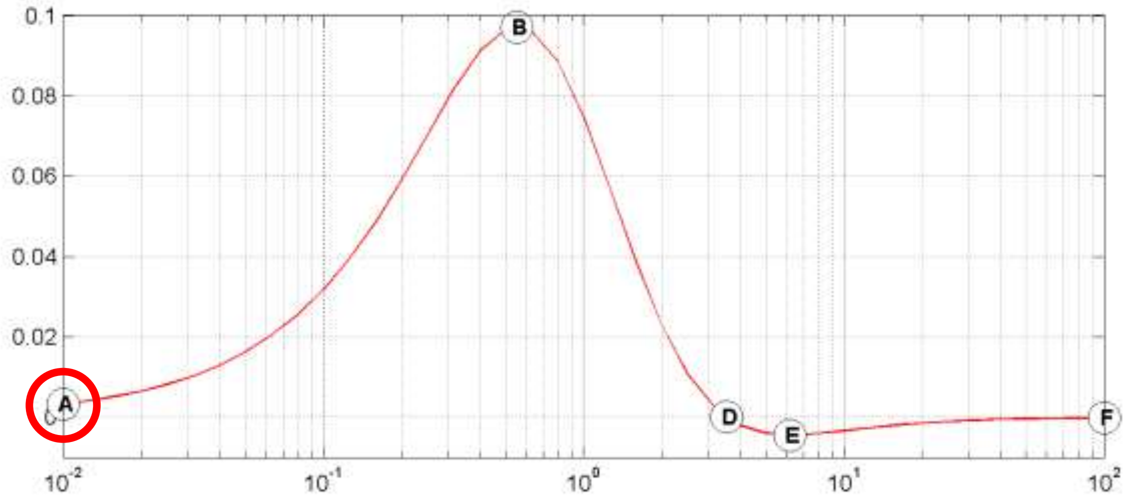
Net velocity characteristics – low frequencies

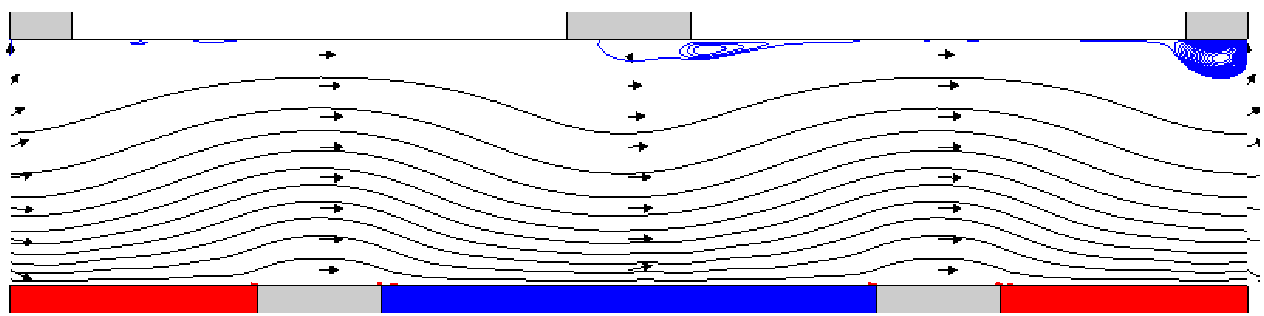


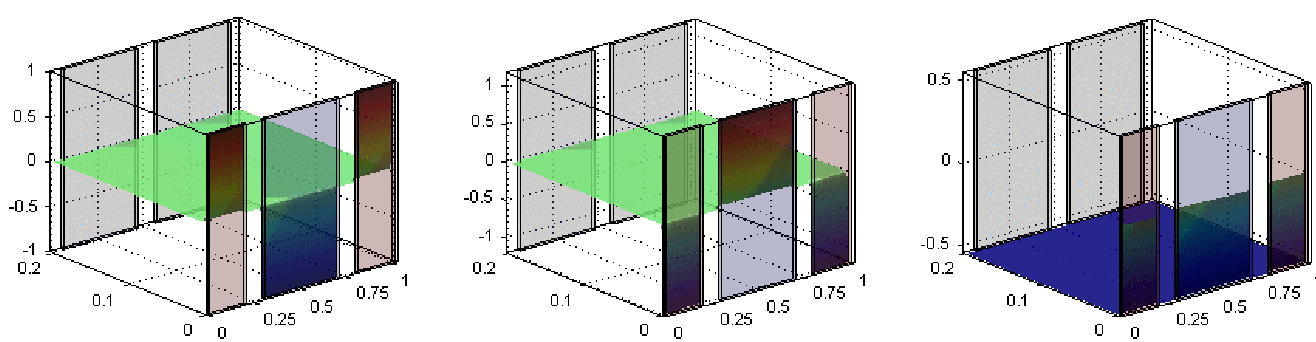
$$\tilde{A} = 1, \quad c_\circ = 92.54\,\mathrm{mol/m^3}, \quad \tilde{\lambda}_D = 0.001 \quad \rightarrow \quad L = 1\,\mu\mathrm{m},\, f_\circ = 2\,\mathrm{MHz}$$

$$\lambda_D = \sqrt{\frac{\varepsilon RT}{2c_\circ F^2}} \quad \& \quad c_\circ = \frac{\varepsilon RT}{2\lambda_D^2 F^2}$$

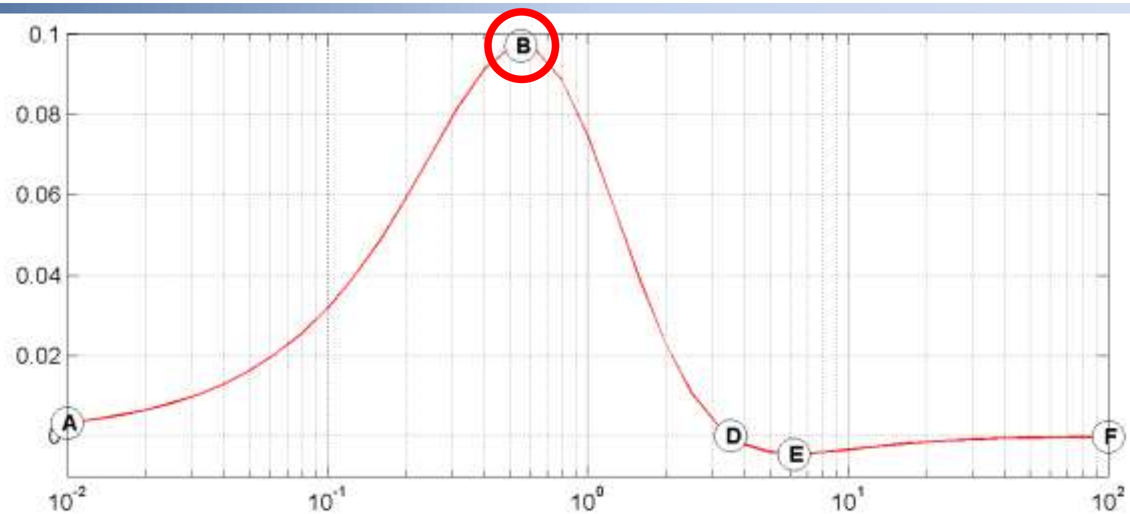
Net velocity characteristics – low frequencies

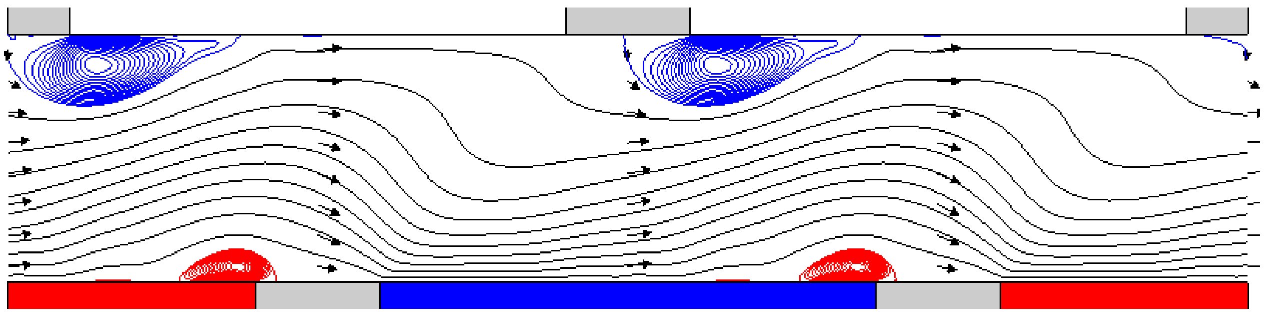


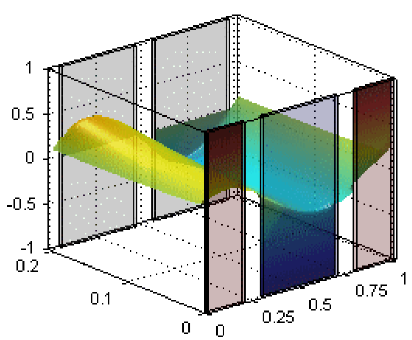


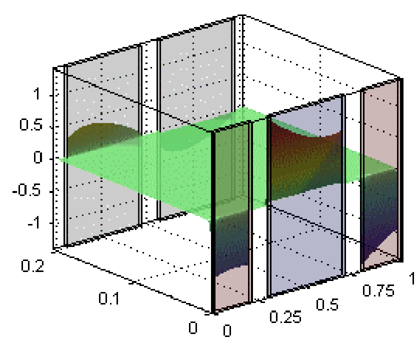


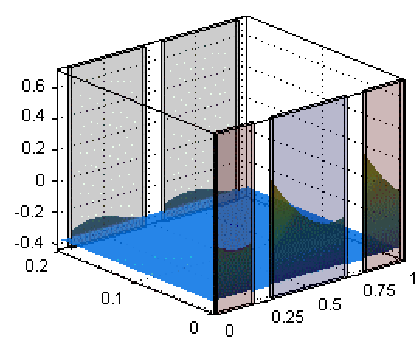
Net velocity characteristics – forward regime



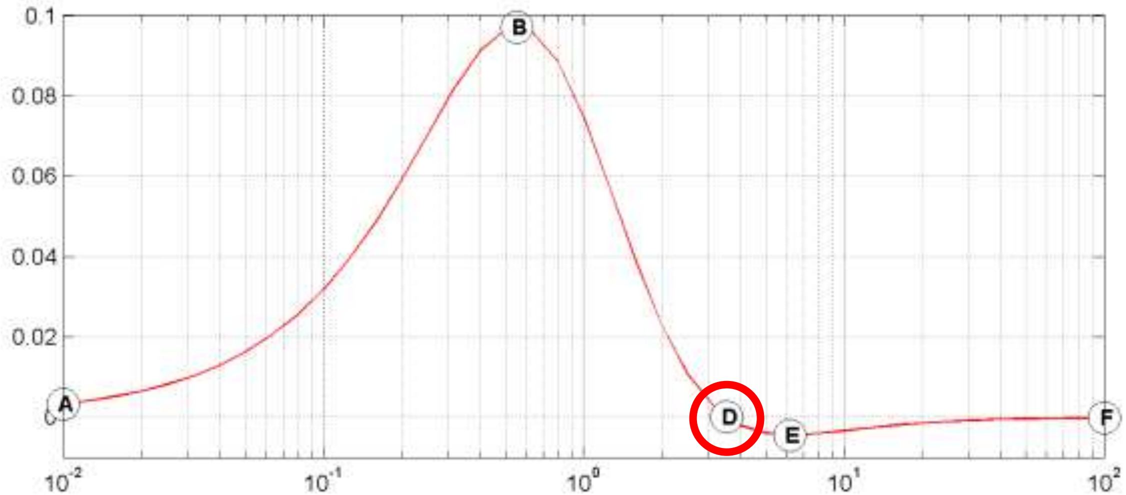


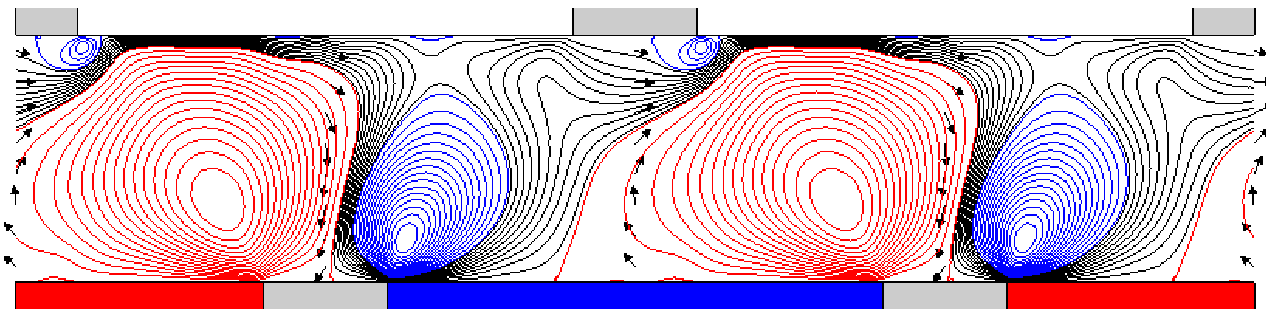


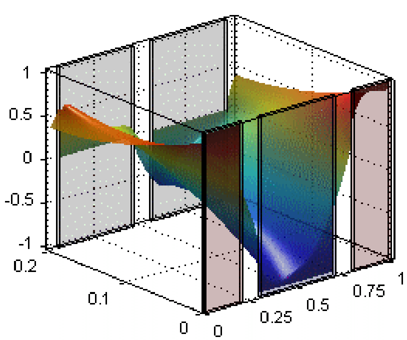


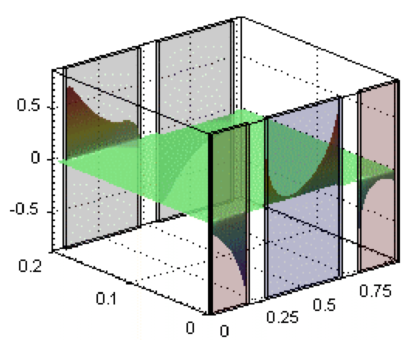


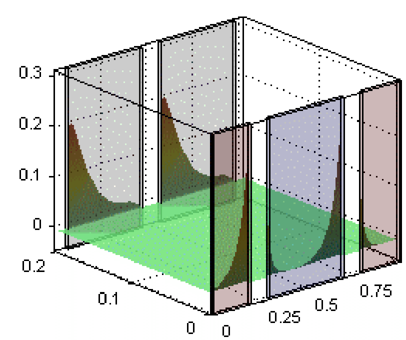
Net velocity characteristics – point of reversion



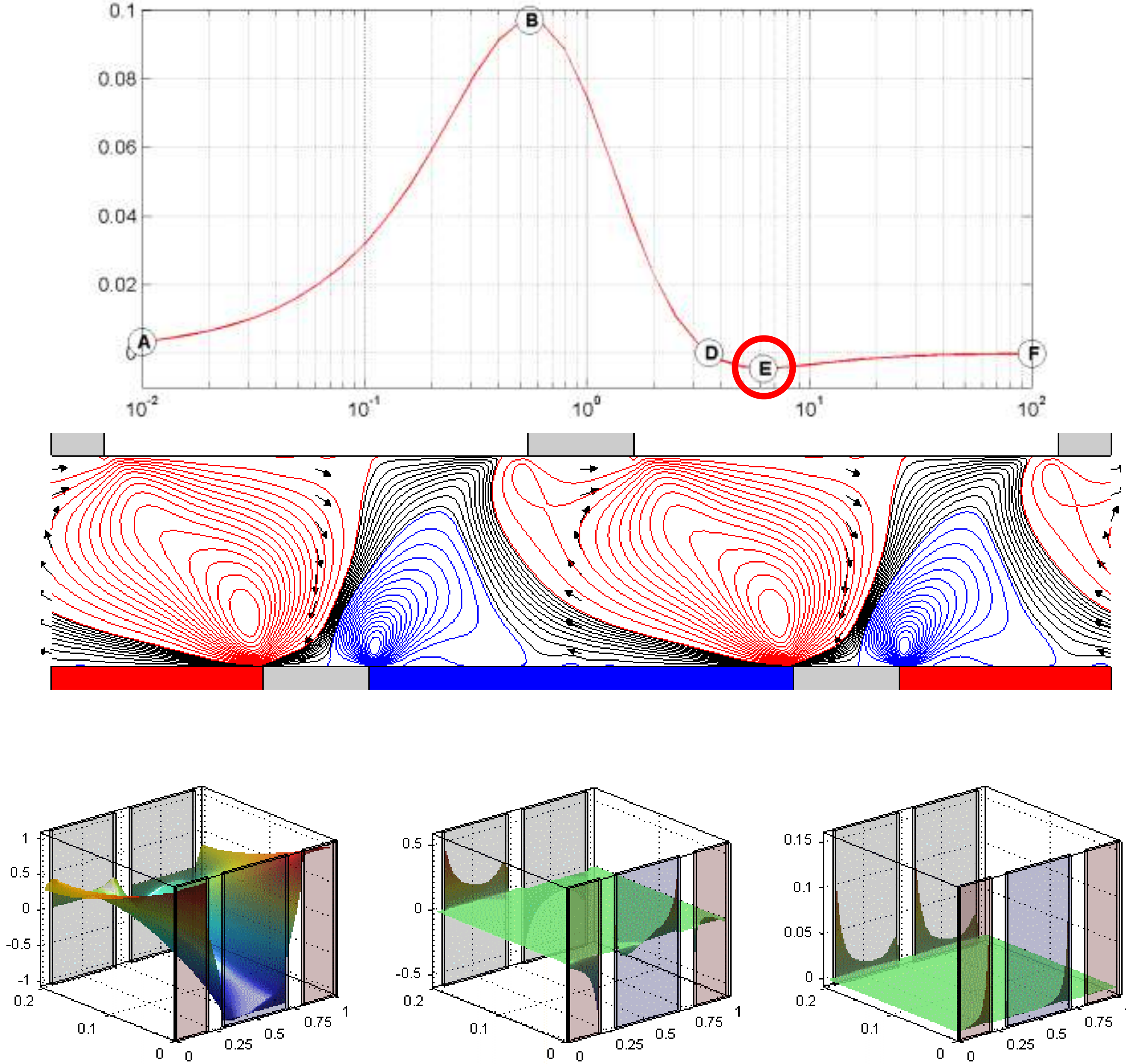




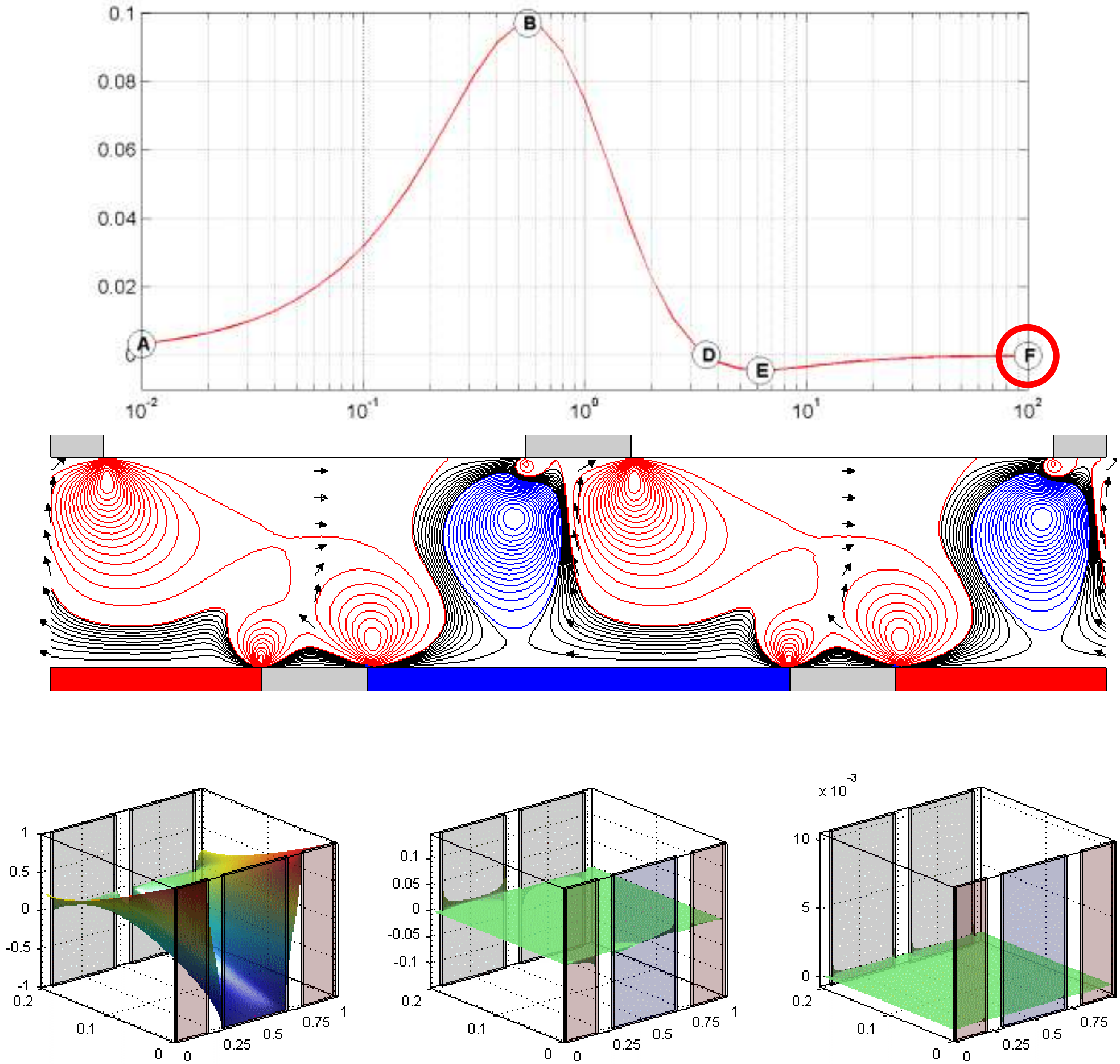




Net velocity characteristics – reversed regime



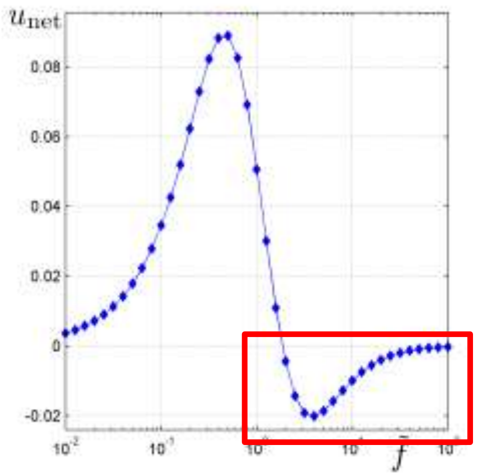
Net velocity characteristics – high frequencies

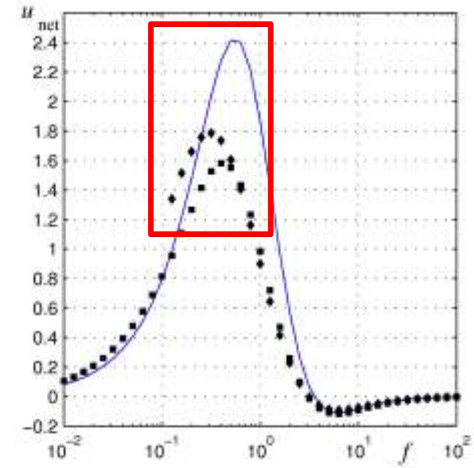


Conclusions

Zig-zag arrangement seems to have promising features

- Employs an interdigital technique for easier electrode arrays construction
- The electrode overlap makes posibility to control the flow direction





- The further miniaturization positively influences the net velocity

$$u_\circ = \frac{D}{L}$$

Future directions

- Experimental realization (first steps)
- More accurate model of EDL is needed (condensed layer), nonlinear description
- Incorporation of the energy balance to our mathematical model

Questions & Answers

Thank you for your attention!

Frequently Asked / Anticipated Questions:

- Continuum hypothesis vs. small elements
- Experimental realization
- Discretization mesh validation
- Cap height estimation
- Periodic regime determination