The Abdus Salam
International Centre for Theoretical Physics

United Nations
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World Year of PHYSICS 2005

SMR.1670 - 5

INTRODUCTION TO MICROFLUIDICS

8 - 26 August 2005

Numerical Methods for Micro Fluidics

Electrokinetically Driven Liquid Micro Flows

A. Beskok
Texas A&M University, U.S.A.

Numerical Modeling Challenges

- Multi Physical Phenomenon (Thermal, Fluidic, Mechanical, Biological, Chemical, Electrical)
- Multi Scale (Atomistic, Continuum)
- Complex Geometry

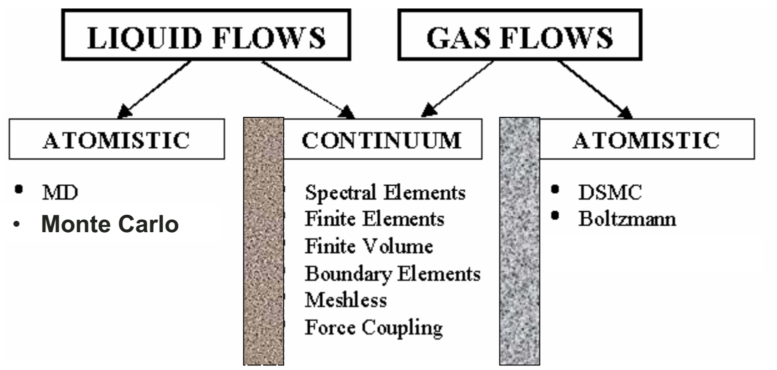
Numerical Simulation Strategies

Scientific Simulations:
- Multi Scale
- Simpler Geometry
- Accurate (error < 1 %)

Engineering Simulations:
- Multi Scale
- Multi Physics
- Complex Geometry
- Accurate (error < 5~10 %)

Low Order Models:
- Multi Physics
- Full Device Simulation
- Lower Accuracy, but Fast (error ~10 %)

Numerical Methods for Micro Fluidics



Mesoscopic:
- Lattice Boltzmann
- Dissipative Particle Dynamics

…

Continuum Simulations with FEM, SM and SEM

- Similarities: Method of Weighted Residual

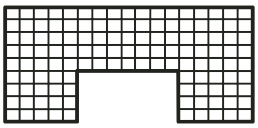
$$\nabla^2 u - f = 0 = \text{Residual} \quad R$$

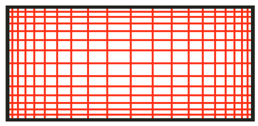
$$u(x,y) \approx u_N(x,y) = \sum_{i=0}^{N} \hat{u}_i S_i(x,y)$$

$$\iint_{\Omega} R_N w d\Omega = 0$$

- Differences: domain and elemental discretizations

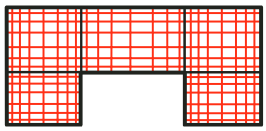
Finite Element Method





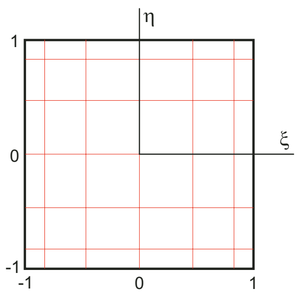
Spectral Method

Spectral Element Method



FEM & SEM

- The difference is the choice of the *basis functions*.
  - **Classical FEM (h-FEM)** uses low-order interpolation functions.
  - **p-FEM** provides high-order approximations through the use of hierarchical basis functions.
  - **SEM** uses high-order Lagrange interpolants based on *Jacobi polynomials.*



$$u_N^e(\xi,\eta) = \sum_{m=1}^{N}\sum_{n=1}^{N} u_{mn}^e \, l_m^N(\xi) l_n^N(\eta)$$

$$l_m^N(\xi) = -\frac{(1-\xi^2)L_N'(\xi)}{N(N+1)L_N(\xi_m)(\xi-\xi_m)}$$

Gauss Lobatto Points

Advantages of High Order Discretizations

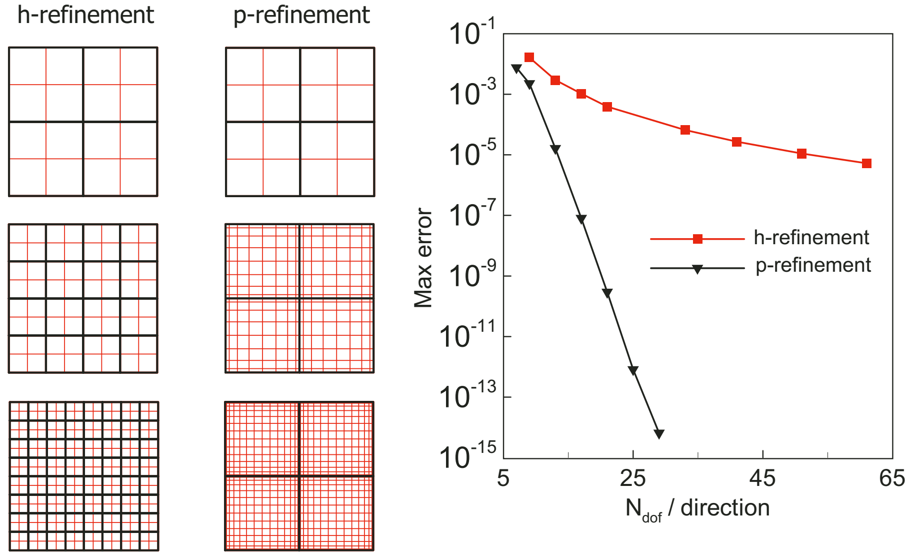
- Fast Convergence, e.g. *exponential error decay*
- Minimum Diffusion/Dispersion errors
- Better skew mesh tolerance
- Smaller volume of data ⟶ Better I/O
- Greater volume/surface ratio ⟶ efficient parallel computing
- Inf-sup condition in Navier-Stokes is better satisfied
- Locking effects in solid mechanics are avoided

Disadvantages

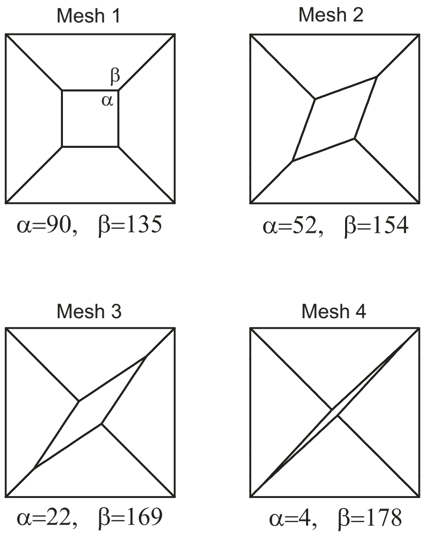
- Discontinuities in the solution leads to loss of convergence and *Gibbs* phenomena

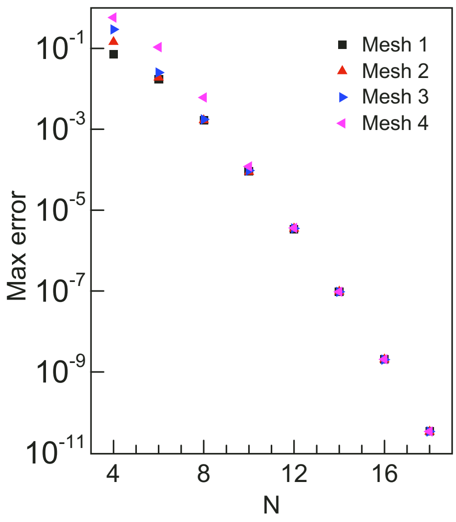
- Large elements limit geometric discretization flexibility
  ⟶ **unstructured & nonconforming formulations**

Spectral vs Algebraic Convergence



Skew mesh tolerance



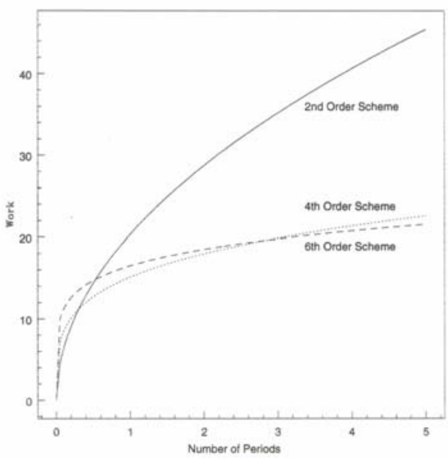


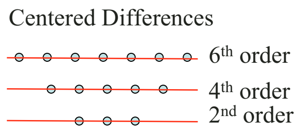
Phase Error Characteristics

Long time integration of unsteady flows:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

- Model problem is a wave equation
- Advect waveform for M time periods
- Computational work W, to maintain *phase error* ε below 10% as a function M



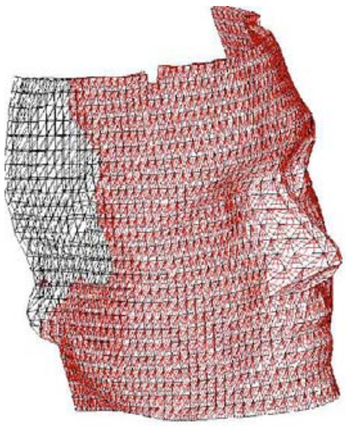


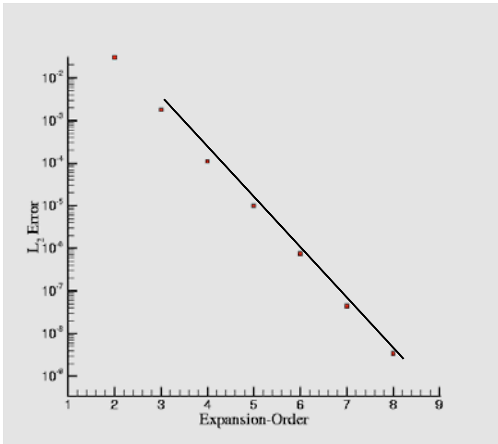
$$W^{(2)} = C_2 \varepsilon^{-1/2} M^{1/2}$$

$$W^{(4)} = C_4 \varepsilon^{-1/4} M^{1/4}$$

$$W^{(6)} = C_6 \varepsilon^{-1/6} M^{1/6}$$

Unstructured SEM:
Geometric Flexibility w/ High Order Resolution

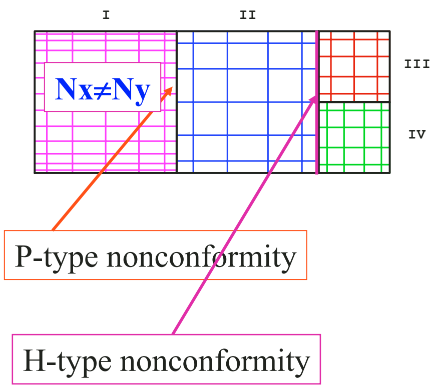


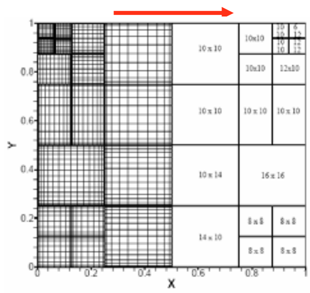


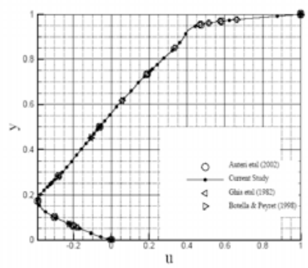
An Unstructured H/P Spectral Method: *Νεκταr*

Nonconforming SEM:
Localized Refinements

Constrained element & Mortar element methods

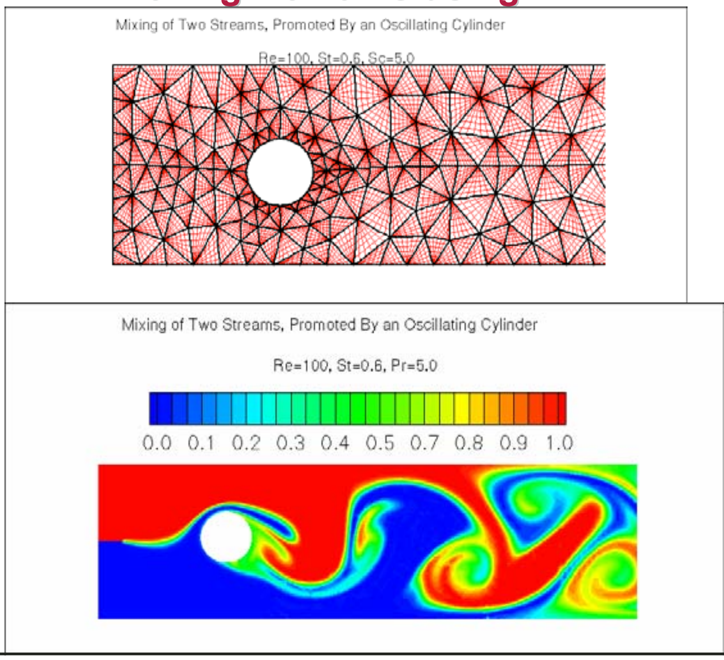


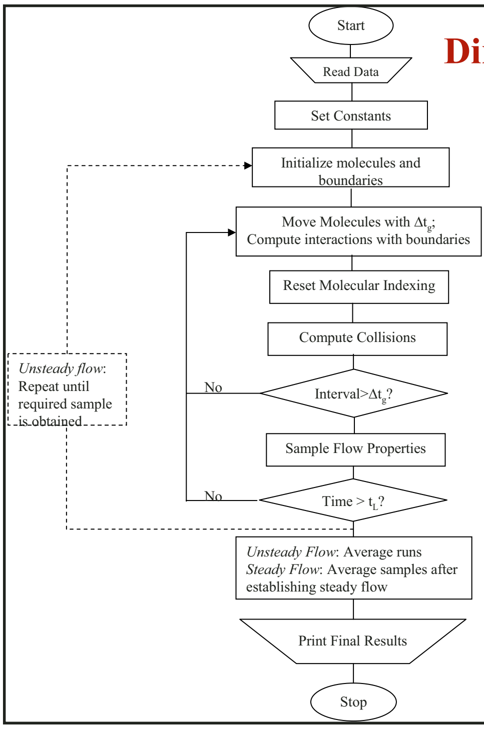




Sert & Beskok, Journal of Computation Physics, 2005

Moving Domains using ALE





Direct Simulation Monte Carlo (DSMC)

Main Steps:

- Particle motion (with $\Delta t < \Delta t_c$)
- Indexing & cross referencing of particles
  Find new cell locations of the molecules
- Simulation of collisions
- Sampling of macroscopic properties

Direct Simulation Monte Carlo (DSMC)

Limitations:

1. Finite Cell Size: $$\mu = \frac{5}{16d^2}\sqrt{\frac{mk_bT}{\pi}}\left[1+\frac{16}{45\pi}\frac{\Delta x^2}{\lambda^2}\right]$$

2. Finite Time Step: $$\mu = \frac{5}{16d^2}\sqrt{\frac{mk_bT}{\pi}}\left[1+\frac{16}{75\pi}\frac{v_m^2\Delta t^2}{\lambda^2}\right]$$

3. Ratio of simulated molecules to the real molecules
(If too low increases statistical scatter)

4. Boundary Condition (Inflow/Outflow)

5. Uncertainties in the Physical Input Parameters
(input for HS, VHS, VSS models)

DSMC Method Disadvantages:

- **Slow Convergence:**

$$\varepsilon \propto \frac{1}{\sqrt{n}}$$

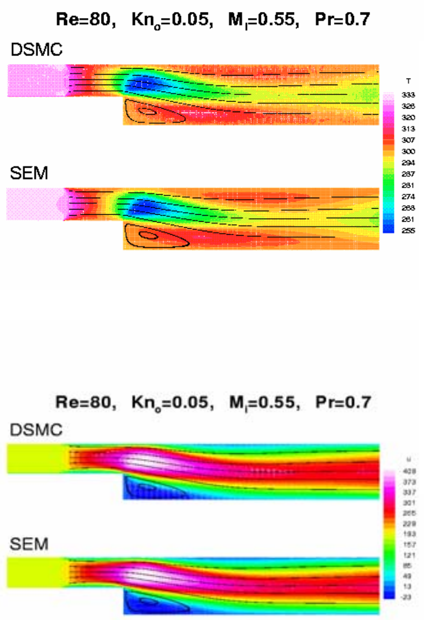
- **Large Statistical Error:**

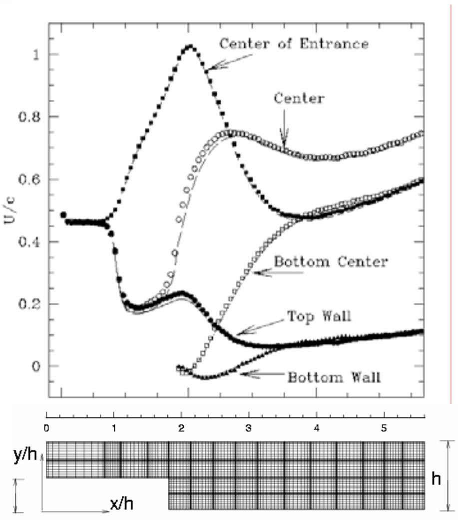
($\sim 10^8$ samples)

- **Extensive Number of Particles:**

3 cells per λ
20 particles per cell

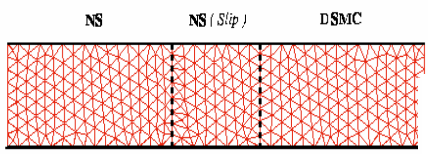
Comparisons of Molecular versus Continuum Solutions

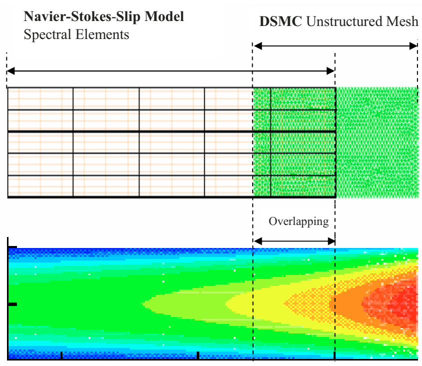




Multi-Domain Simulation: DSMC/Continuum Coupling

- Hash & Hassan (1995)
- Garcia et al. (1999)
- Hadjiconstantinou (1999)
- Liu (1999)
- Aluru (2001)

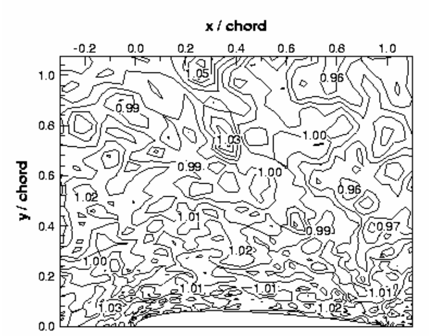




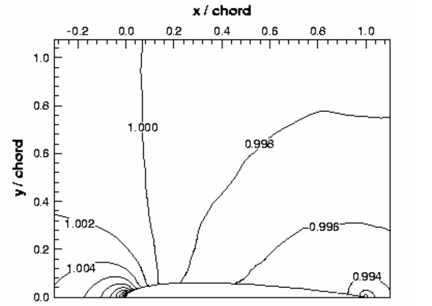
Hand-Shake Region

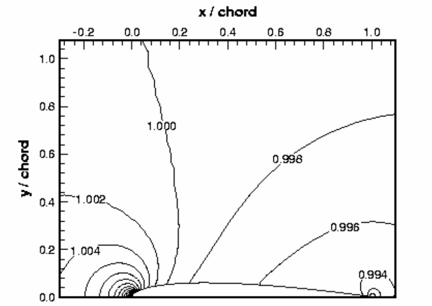
- Zanolli iterative patching

New Developments: Information Preservation DSMC



(a) DSMC





(c) Continuum approach with a slip boundary condition

Density contours for
M=0.1, Re=1, Kn=0.013 Flow

Courtesy of I. Boyd

Electrokinetically Driven Liquid Micro Flows

Ali Beskok

Texas A&M University
Mechanical Engineering Department

College Station, TX 77845
abeskok@tamu.edu

Microfluidics:

Emerging technology that allows development of new approaches to synthesize, purify, and rapidly screen chemicals, biologicals, and materials using integrated, massively parallel miniaturized platforms.

- Microfluidics is *interdisciplinary*:
  - Micro-Fabrication
  - Chemistry
  - Biology
  - Mechanics
  - Control Systems
  - Micro-Scale Physics and Thermal/Fluidic Transport
  - Numerical Modeling
  - Material Science
  - System Integration and Packaging
  - Validation & Experimentation
  - Reliability Engineering
  - …

Microfluidic Devices

Sensors & Actuators:

Pressure, Temperature, Shear Stress, Biological & Chemical Sensors

Fluidic Components:

Channels, Pumps, Membranes Valves,
Nozzles, Diffusers and Mixers

Motion Generation:

Micro-Motors, Turbines,
Steam Engines, Gears, Pistons, Links

Microfluidic Applications:

Defense Applications:

- Lab on a chip: μ-TAS

Bio-Medical Applications:

- Drug Delivery Systems
- DNA Analyzers
- Human Health Monitoring
- Artificial Organs

Environmental Monitoring:

- Water & Air Pollution Sensing
- Gas/Liquid Filtration Systems

Microelectronics:

- Thermal Management
- Bubble-Jet Printers

Aerospace Industry:

- Drag & Stall Control

Physical Challenges of Micro-Scale Transport

- *Gas Flows*
  - Compressibility
  - *Rarefaction*
    - Slip
    - Transition
    - Free Molecular
    - Thermally Induced Motion
  - Surface & Roughness
  - Viscous Heating
  - Incomplete Similitude
  - …
- *Liquid Flows*
  - Wetting
  - Adsorption
  - Slip
  - *Electrokinetics*
  - Polarity
  - Coulomb & van der Waals Forces
  - Capillary Forces
  - Roughness
  - …

Constitutive Laws, Boundary Conditions, Surface, Interface and Body Forces

Liquid Flows

- **Electrokinetic Transport:**
  - **Electric Double Layer (EDL)**
  - **Electroosmosis (Steady, AC, Time-Periodic)**
  - **Electrophoresis (& Dispersion)**
- **Dielectrophoresis (AC/DC)**

Incompressible Flow with Electrokinetic Forces

$$\nabla \cdot \vec{u} = 0 \qquad \text{(Continuity)}$$

$$\rho_f \left(\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} \right) = -\nabla P + \mu \nabla^2 \vec{u} + \vec{F}_{EK} \qquad \text{(N.S.)}$$

$$\vec{F}_{EK} = \rho_q \vec{E} - \frac{1}{2} \vec{E}^2 \nabla \varepsilon + \frac{1}{2} \nabla \left(\rho_f \frac{\partial \varepsilon}{\partial \rho_f} \vec{E}^2 \right) \qquad \text{(EK force in liquid)}$$

Ignored in incompressible fluid

Permittivity variations
with density→ important at
gas/fluid interface
also for gas flows

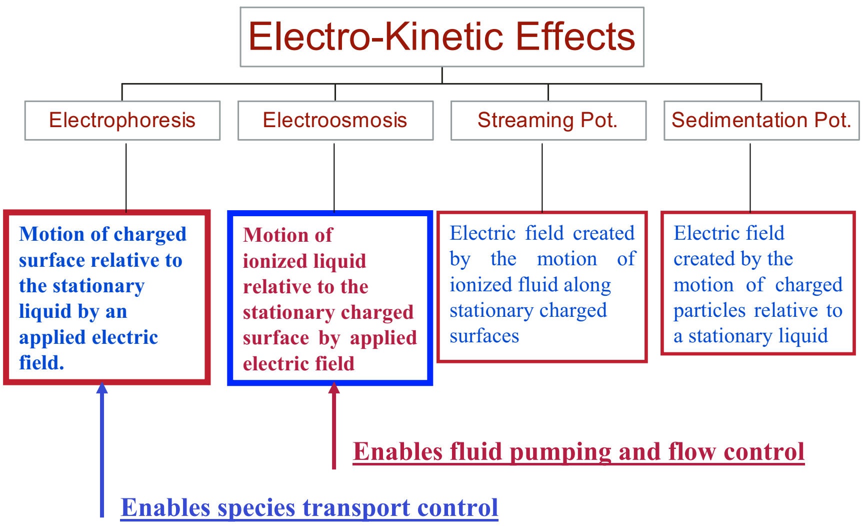
Species Conservation Equation

(for i^{th} species)

$$\frac{\partial c_i}{\partial t} + \nabla \vec{j}_i = 0$$

$$\vec{j}_i = -D_i \nabla c_i + \left[c_i \vec{u} + c_i \mu_{ek,\,i} \vec{E} \right]$$

Diffusion — Convection due to bulk fluid flow — Transport due to EK mobility



Other Microfluidic Particle Sorting & Separation Techniques

Isoelectric focusing is the migration of charged particles under pH gradients to a location in the buffer, where they have zero net charge

Dielectrophoresis is the motion of polarizable particles that are suspended in an electrolyte and subjected to a spatially non-uniform electric field. The particle motion is produced by the dipole moments induced on the particle and the suspending fluid.

Concept of Electric Double Layer (EDL)

Poisson-Boltzmann Equation

$$\nabla^2 \psi = -\frac{4\pi\rho_q}{D}$$

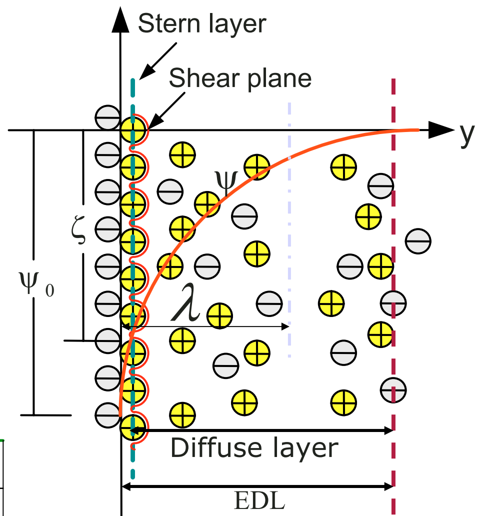
$$\rho_q = -2n_o ez \sinh(ez\psi / k_b T)$$

↑ Boltzmann Distribution

$$\alpha = ez\zeta / k_b T$$

$$\omega = \frac{1}{\lambda} = \sqrt{\frac{8\pi n_o e^2 z^2}{D k_b T}}$$

n_0 [M]	λ [nm]
1e-2	3
1e-5	100
1e-6	300



- ζ on the surface is negative
- ζ on the liquid side is positive

New Equations

$$\nabla^2\psi = -\frac{4\pi\rho_e}{D}$$

$$\rho_e = -2n_o ez\sinh(ez\psi / k_b T)$$

$$\alpha = ez\zeta / k_b T$$

$$\omega = \frac{1}{\lambda} = \sqrt{\frac{8\pi n_o e^2 z^2}{Dk_b T}}$$

$$\beta = (\omega h)^2 / \alpha$$

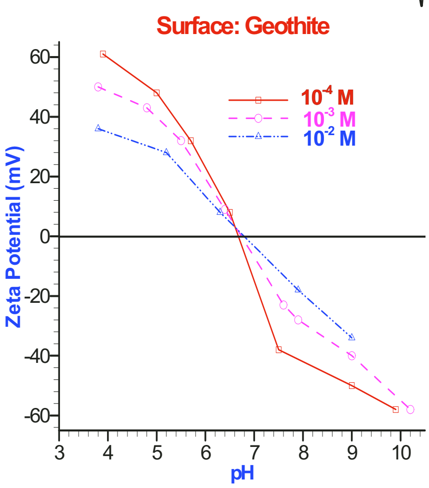
$$\nabla^2\psi^* = \beta\sinh(\alpha\psi^*)$$

Nomenclature

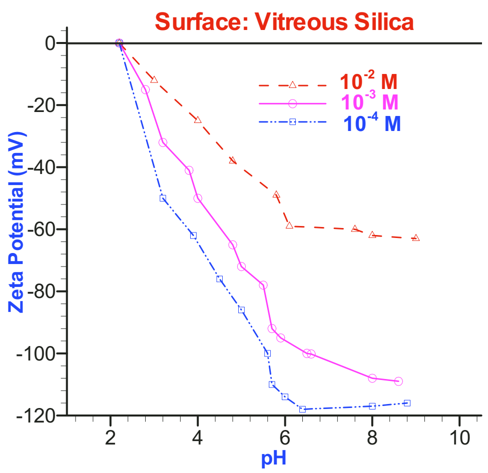
D	Dielectric constant
e	electron charge
k_b	Boltzmann constant
n_o	ion concentration
z	valence
α	ionic energy parameter
ε	$D/4\pi$
λ	Debye length
ρ_e	electric charge density
ϕ	electric field potential
ψ	electroosmotic potential
ω	Debye-Hückel parameter $1/\lambda$
ζ	zeta potential

Zeta Potential of Surface-Liquid Interface

$$\alpha = ez\zeta / k_b T \qquad \omega = \sqrt{\frac{8\pi n_o e^2 z^2}{Dk_b T}} \qquad \beta = (\omega h)^2 / \alpha$$



Source: Fuerstenau and Healy, 1972



Source: Wiese et al., 1971

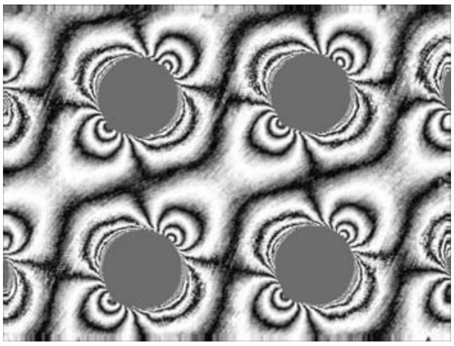
Electroosmosis

Motion of ionized liquid relative to the stationary charged surface by applied electric field

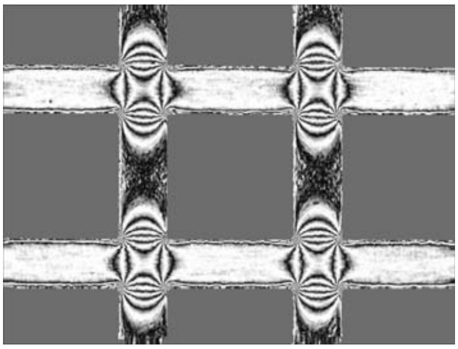
Typical Parameters for EO Flow

Parameter	Parameter range
Typical channel thickness, h (μm)	$0.01 \sim 300$
Electrolyte concentration, n_o (mM)	$10 \sim 0.001$
Debye length, λ_D (nm)	$1 \sim 100$
Zeta potential, ζ (mV)	$\pm 1 \sim \pm 100$
Electric field, $\mathbf{E}$ (V/mm)	$1 \sim 100$
Electroosmotic Velocity, U (mm/s)	< 2
Reynolds number, Re	$10^{-4} \sim 1$

Electroosmotic Flow: Experimental Results in Complex Geometries



Speed contours in an array of posts at 45° wrt the applied electric field 2V/mm



Streamwise velocity contours. Applied electric field 1V/mm from left to right

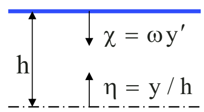
Micro-PIV results presented in the form of simulated interferogram
Courtesy of E. Cummings

EO Potential:

Analysis of 1-D Poisson-Boltzmann Equation

(a) Poisson-Boltzmann Equation in 1-D

$$\frac{d^2\psi^*}{d\eta^2} = \beta \sinh(\alpha\psi^*)$$



(b) Derivative of the Electroosmotic Potential

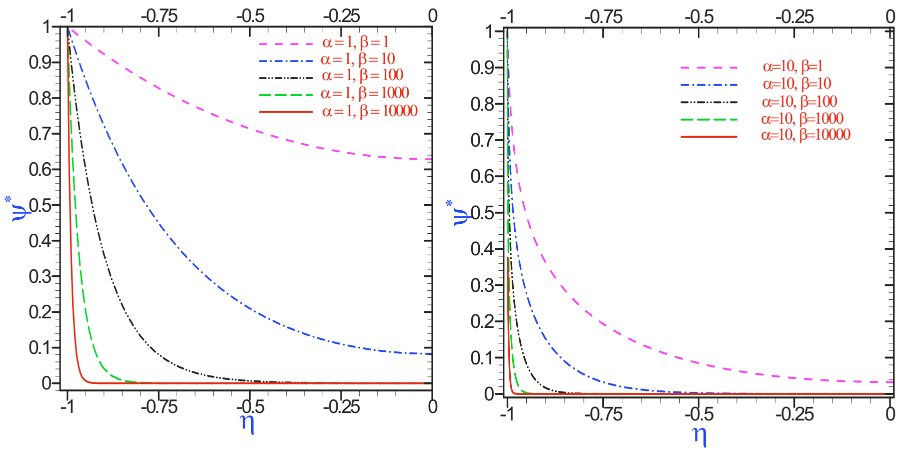
$$\frac{d\psi^*}{d\eta} = \sqrt{\frac{\beta}{\alpha}}\sqrt{2\cosh(\alpha\psi^*) - 2\cosh(\alpha\psi_c^*)}$$

(c) Potential Distribution across the Channel

$$\psi^* = \frac{4}{\alpha}\tanh^{-1}\left[\tanh\left(\frac{\alpha}{4}\right)\exp\left(-\sqrt{\alpha\beta}\,\eta^*\right)\right]$$

$$\chi = \sqrt{\alpha\beta}\,\eta^* \qquad \chi = \omega y' = \omega h(1-\eta)$$

Potential Distribution Across the Channel



$$h/\lambda = \sqrt{\alpha\beta}$$ This is a measure of EDL thickness relative to the channel height

Dutta & Beskok *Analytical Chemistry*, 73(9); 1979-1986, 2001.

Incompressible Flow with Electro Kinetic Forces

$$\nabla \cdot \vec{u} = 0$$ (Continuity)

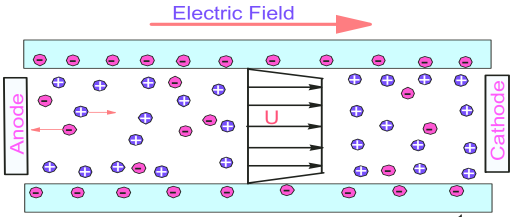
$$\rho_f \left(\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} \right) = -\nabla P + \mu \nabla^2 \vec{u} + \vec{F}_{EK}$$ (N.S.)

$$\vec{F}_{EK} = \rho_q \vec{E}$$ (EK Force)

$$\rho_q = -2n_o ez \sinh(ez\psi / k_b T)$$
$$\nabla^2 \psi = -\frac{4\pi \rho_q}{D}$$
(Poisson Boltzmann Equation)

$$\nabla^2 \phi = 0$$
$$\vec{E} = -\nabla \phi$$
(External Electric Field)

Pure Electroosmotic Flow in a Channel

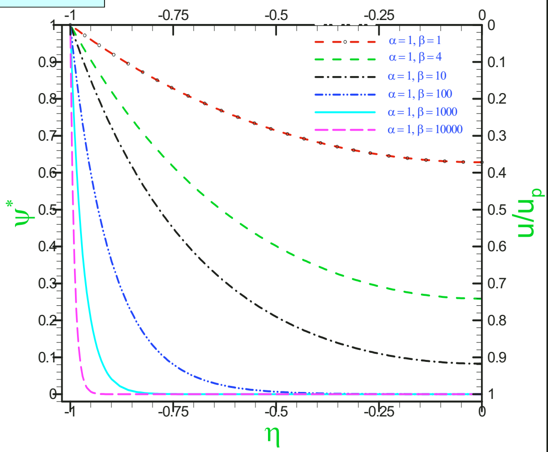


$$\frac{\partial P^*}{\partial \xi} = \frac{d^2 U}{d\eta^2} + \frac{d^2 \psi^*}{d\eta^2}$$ (with $\frac{\partial P^*}{\partial \xi}$ crossed out → 0)

$$\mathrm{U} = \mathrm{u} / \mathrm{u_p} = 1 - \psi^*$$

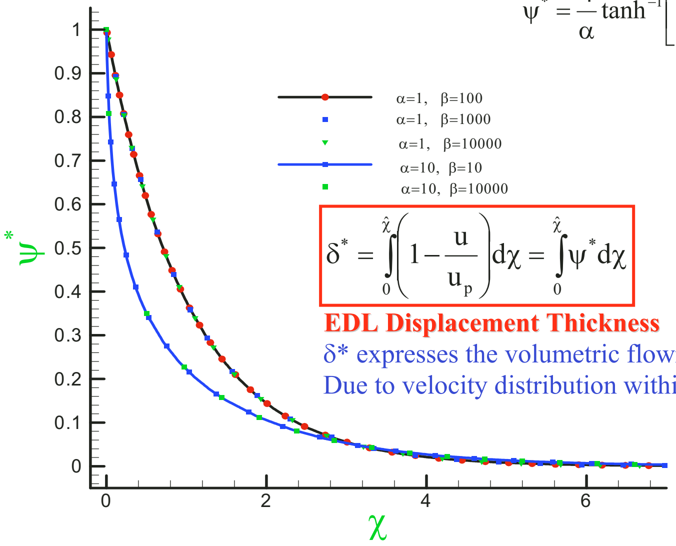
$$u_p = -\frac{\zeta \varepsilon \vec{E}}{\eta}$$

↑ Helmholtz-Smoluchowski Velocity



Potential Distribution Near the Wall

$$\psi^* = \frac{4}{\alpha}\tanh^{-1}\left[\tanh\left(\frac{\alpha}{4}\right)\exp(-\chi)\right]$$



$$\psi^* = \left(1 - \frac{u}{u_p}\right)$$

$$U = 1 - \psi^*$$

$$\chi = \omega y$$

$$\delta^* = \int_0^{\hat{\chi}} \left(1 - \frac{u}{u_p}\right) d\chi = \int_0^{\hat{\chi}} \psi^* d\chi$$

EDL Displacement Thickness

δ^* expresses the volumetric flowrate defect

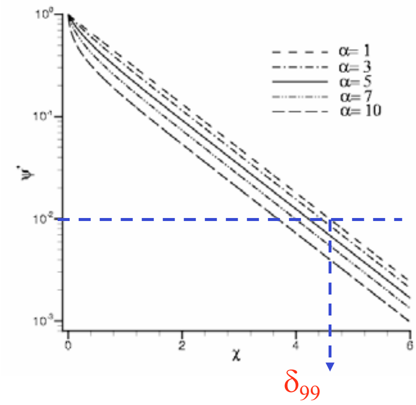
Due to velocity distribution within the EDL

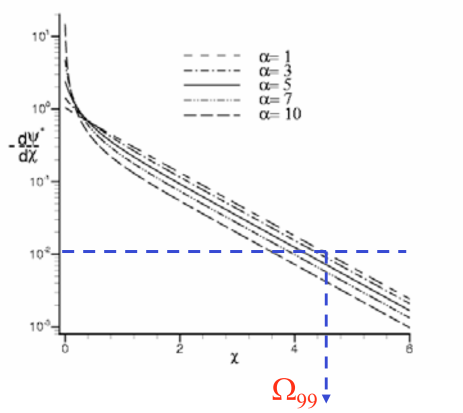
Dutta & Beskok *Analytical Chemistry*, 73(9); 1979-1986, 2001.

New Concepts in Electroosmotic Flows
Analogy to Boundary Layer Theory

Effective EDL Thickness δ_{99}

EDL Vorticity Thickness Ω_{99}

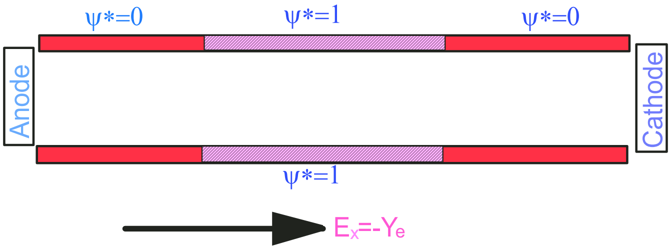




$$\chi = \omega y$$

Dutta & Beskok *Analytical Chemistry*, 73(9); 1979-1986, 2001.

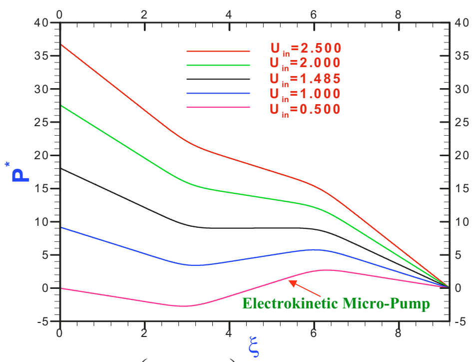
Mixed Electroosmotic/Pressure Driven Channel

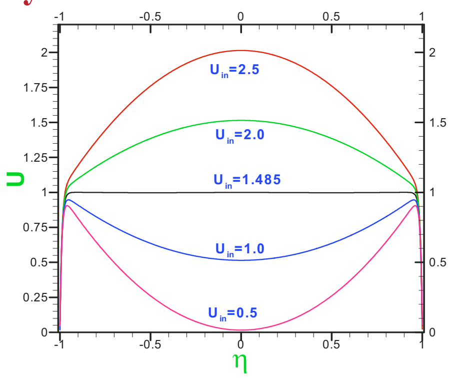


- Electroosmotic flow is present in the mid part of the channel.
- Various inlet conditions (flowrate) are specified to obtain mixed electroosmotic/pressure driven flow.
- Simulations are for α=1, β=10,000, Re=0.005 flow
- The EDL is resolved

TAMU Micro Fluidics Laboratory

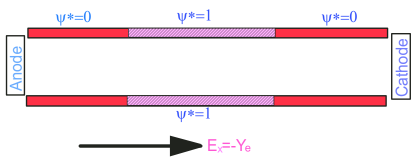
Mixed Electroosmotic/Pressure Driven Channel
Pressure & Velocity Distributions





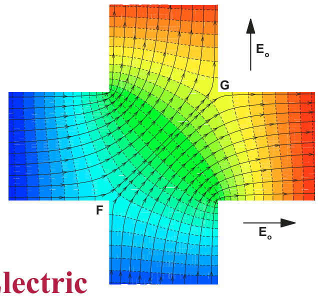
$$\frac{dP^*}{d\xi} = 3\left(1 - \frac{\delta^*}{\sqrt{\alpha\beta}}\right) - 2U_{in} \qquad U_{in} = \frac{u_{max}}{u_p}$$

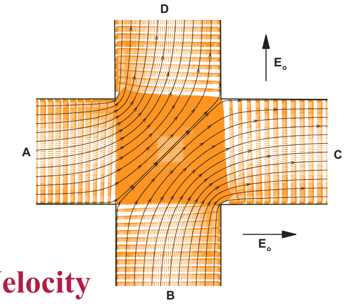
$$U(\eta) = -\frac{1}{2}\frac{dP^*}{d\xi}\left(1-\eta^2\right) + 1 - \psi^*(\eta)$$



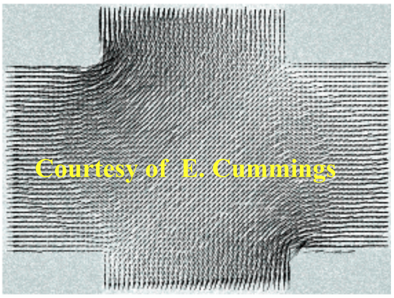
Results are for α=1, β=10,000, Re=0.005

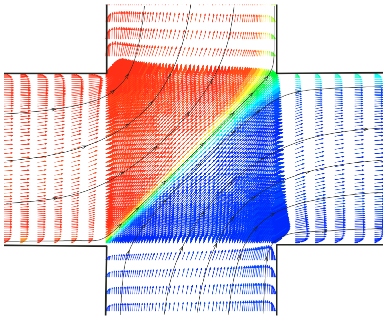
Pure EO Flow in a Cross-Channel



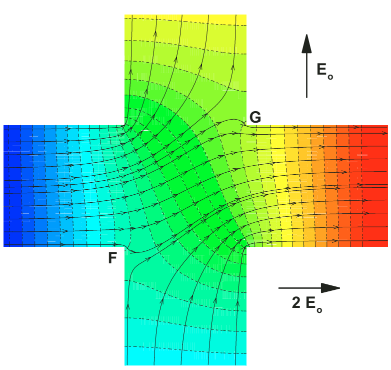


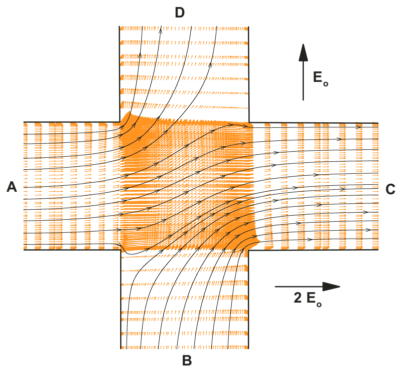
Electric Field → Velocity Field





Electroosmotic Flow *Control* in a Cross-Channel

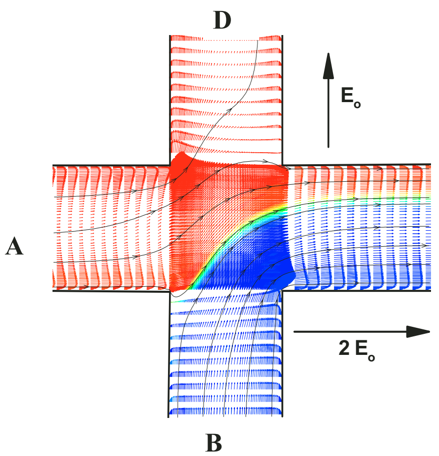


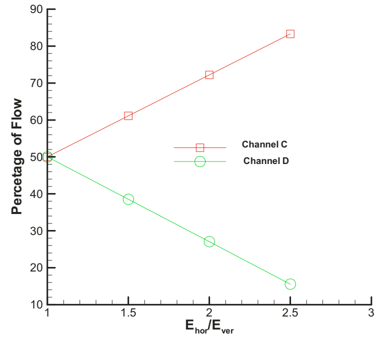


Electric Field → Velocity Field

Dutta, Beskok, Warburton *Journal of MEMS*, **11**(1), 36-44, 2002.

Scalar Transport Control with Mixed Electroosmotic/Pressure Driven Flow:

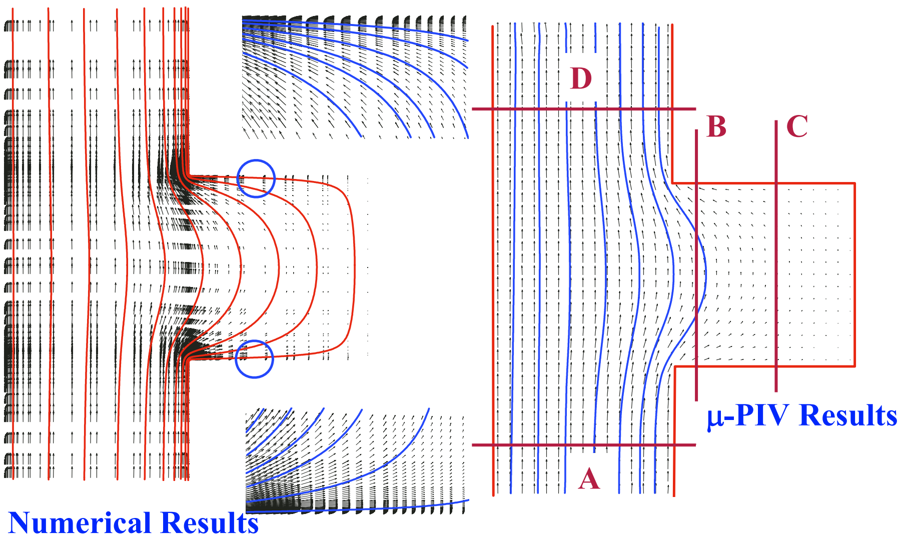




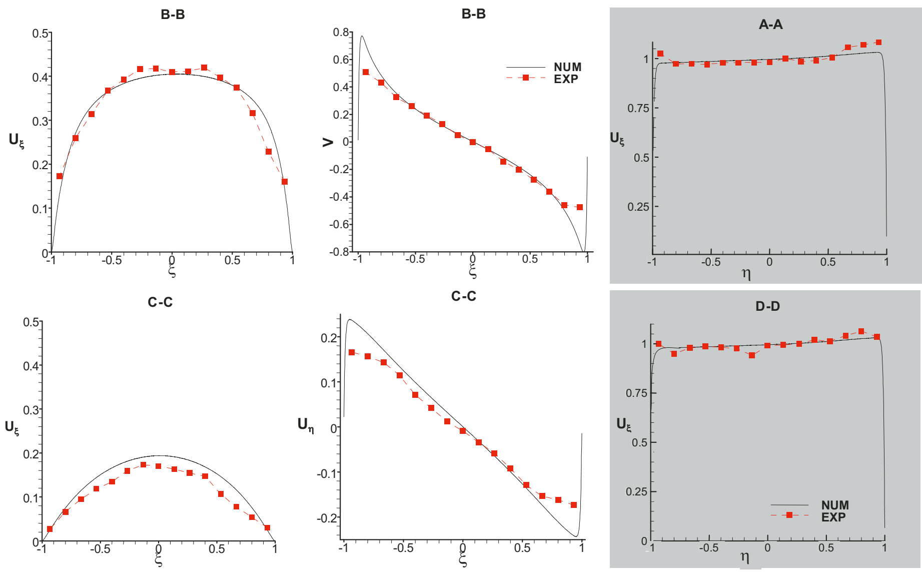
Note that the inlet flowrate in channels A&B are fixed & Equal!

Variations in the ratio of the vertical and horizontal electric field change the flowrate in channels D & C *linearly*. Hence the amount of red fluid in channel C can be controlled!

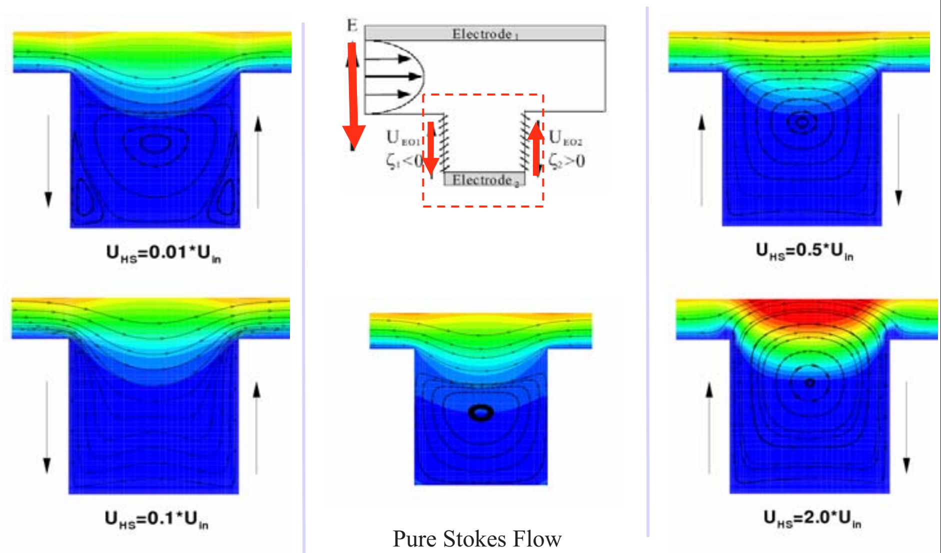
Electroosmotic Flow in a Grooved Channel



Comparison of Numerical Results with μ-PIV in Grooved Channels



Flow Control with Local Electrokinetic Effects



Species Transport in Micro Scales

Despite low Reynolds numbers ($Re \approx 0.01$)
Large particles and bio-molecules have very small mass diffusivities
⟶ large Schmidt numbers and large Peclet numbers

$$Sc = \frac{\nu}{D} \qquad Pe = \frac{UL}{D} \qquad \frac{\text{Diffusion time } (L^2/D)}{\text{Convection time } (L/U)}$$

$$\frac{\partial C}{\partial t} + \vec{U} \cdot \nabla C = \frac{1}{Pe} \nabla^2 C$$

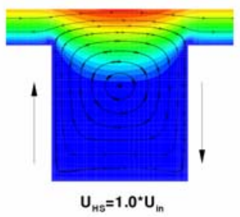
$$Pe \propto 10^3 \sim 10^5$$

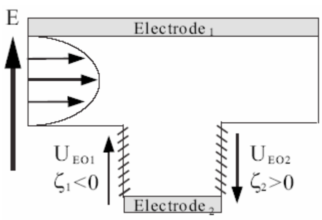
Physical Parameters for large Bio-Molecules

Diffusing Particle in water	Diffusion coefficient (m^2/s)
Red Blood Cell	6.8×10^{-14}
Hemoglobin	7.3×10^{-11}

$\nu_{water} \approx 1.0\times10^{-6}\ m^2/s$

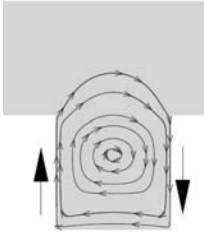
Species Transport Control: Entrapment

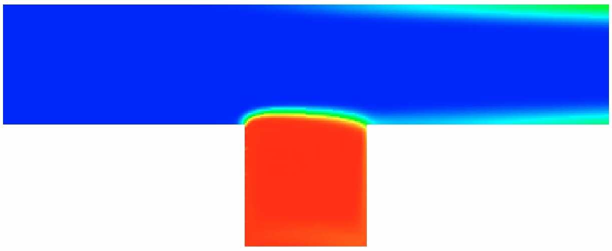




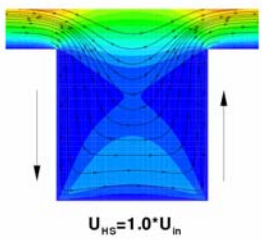
Re=0.005, Pe=1000

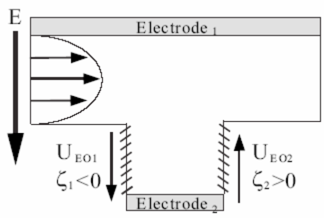
Species Transport Control: Levitation

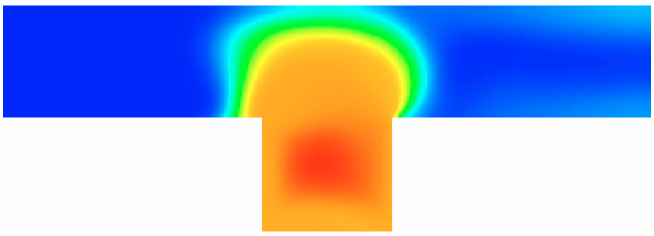




Species Transport Control: Release







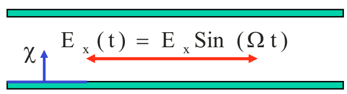
Species Control in Grooved Channel

Using selective surface patterning & local electric fields → entrapment & release of prescribed amounts of scalar species

- Groove size determines the volume of entrapped species
- Each groove can contain one or more species.
- Allows control over the inter-species diffusion and mixing by simple flow kinematics.
- Relatively simple and fast method for combinatorial chemistry experiments in a micro-channel, where multiple species are trapped and released from multiple grooves.

Time Periodic Electroosmotic Flows

$$\rho_f \frac{\partial u}{\partial t} = \mu \frac{\partial^2 u}{\partial y^2} + \rho_e E_x \mathrm{Sin}(\Omega t)$$



$$\rho_e = -2 n_o e z \sinh(e z \psi / k_b T)$$

$$U = \frac{u}{u_p} \qquad u_p = \frac{\zeta \varepsilon Y}{\mu} \qquad \theta = \Omega t \qquad \chi = \frac{y}{\lambda} = \omega y$$

$$\frac{\partial U}{\partial \theta} = \frac{1}{\kappa^2}\left[\frac{\partial^2 U}{\partial \chi^2} + \frac{\mathrm{Sin}(\theta)}{\alpha}\mathrm{Sinh}(\alpha \psi^*)\right]$$

$$\kappa = \frac{\lambda}{h}\sqrt{\frac{\Omega h^2}{\nu}}$$

$$\text{Stokes Number } = \sqrt{\frac{\Omega h^2}{\nu}}$$

Analytical Solution of Time Periodic EO Flow

$$U(\chi,\theta) = \mathrm{Im}[F(\chi).\exp(i\theta)]$$

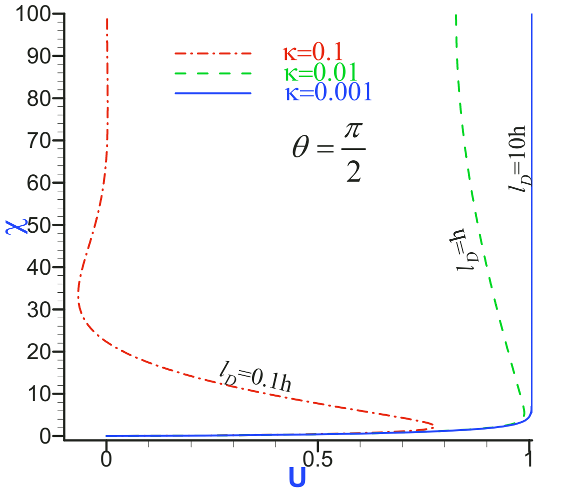
$$\boxed{F(\chi) = 2A\mathrm{Sinh}(\sqrt{i}\kappa\chi) + [C(\chi) - D(\chi)]}$$

$$C(\chi) = \frac{\exp(-\sqrt{i}\kappa\chi)}{2\sqrt{i}\kappa\alpha}\int_0^{\chi}\exp(\sqrt{i}\kappa\chi)\mathrm{Sinh}(\alpha\psi^*)d\chi$$

$$D(\chi) = \frac{\exp(\sqrt{i}\kappa\chi)}{2\sqrt{i}\kappa\alpha}\int_0^{\chi}\exp(-\sqrt{i}\kappa\chi)\mathrm{Sinh}(\alpha\psi^*)d\chi$$

$$A = \frac{\exp(-\sqrt{i}\kappa\chi)\int_0^{\infty}\exp(\sqrt{i}\kappa\chi)\mathrm{Sinh}(\alpha\psi^*)d\chi}{4\sqrt{i}\kappa\alpha\mathrm{Cosh}(\sqrt{i}\kappa\chi)} + \frac{\exp(\sqrt{i}\kappa\chi)\int_0^{\infty}\exp(-\sqrt{i}\kappa\chi)\mathrm{Sinh}(\alpha\psi^*)d\chi}{4\sqrt{i}\kappa\alpha\mathrm{Cosh}(\sqrt{i}\kappa\chi)}$$

Velocity Profiles



$$\kappa = \frac{\lambda}{h}\sqrt{\frac{\Omega h^2}{\nu}}$$

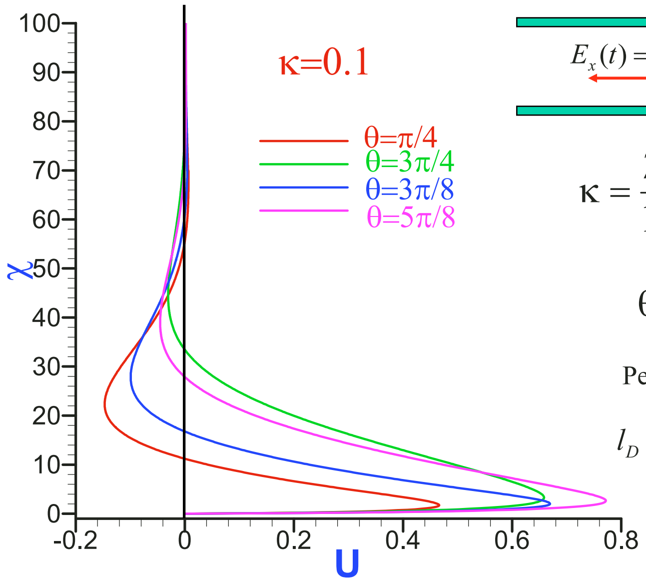
$$h = 100\lambda$$

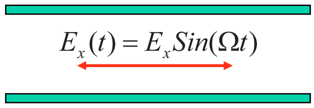
Penetration Depth

$$l_D = \sqrt{\frac{\nu}{\Omega}}$$

•Non-irrotational flows for $l_D < h$

Velocity Distribution as a Function of Time





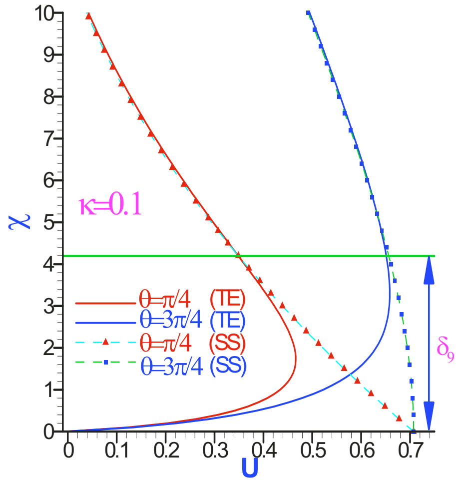
$$\kappa = \frac{\lambda}{h}\sqrt{\frac{\Omega h^2}{\nu}}$$

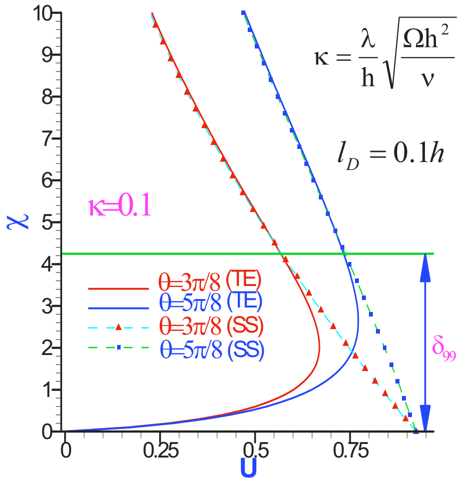
$$\theta = \Omega t$$

Penetration Depth

$$l_D = \sqrt{\frac{\nu}{\Omega}} = 0.1h$$

Near Wall Velocity Profiles: Comparisons to Bounded Stokes Layers

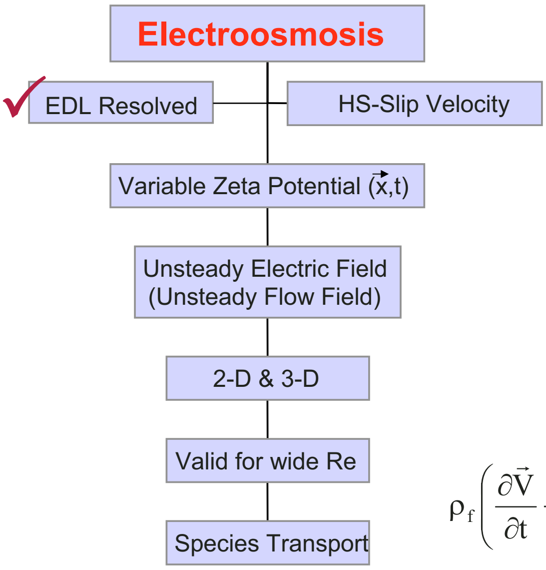




$$\kappa = \frac{\lambda}{h}\sqrt{\frac{\Omega h^2}{\nu}}$$

$$l_D = 0.1h$$

Simplified Modeling Approaches



Electric Field

$$\nabla^2 \phi = 0$$

$$\vec{E} = -\nabla \phi$$

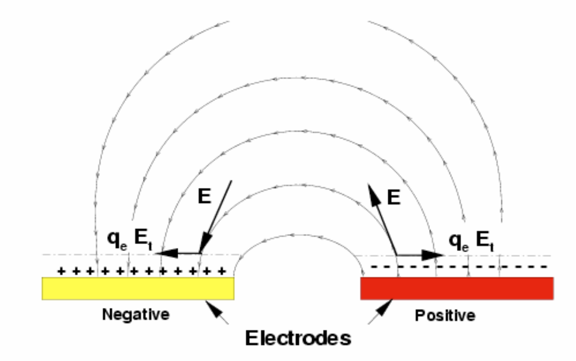
Boundary Condition

$$u_p = \frac{-\zeta \varepsilon \vec{E}}{\mu}$$

Flow Field

$$\rho_f \left(\frac{\partial \vec{V}}{\partial t} + (\vec{V} \cdot \nabla)\vec{V} \right) = -\nabla P + \mu \nabla^2 \vec{V}$$

AC-Electroosmosis

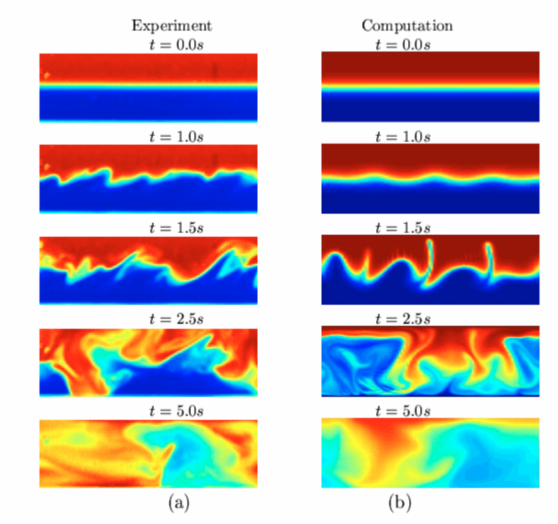


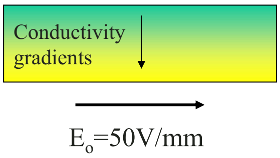
Low Voltages (< 10V)
AC Freq: 10 Hz ~ 100 kHz
Flow rates ~ 1~10 mm^3/s

The flow direction is not changed by reversing the electrode polarity!

See: Morgan & Green, 2003

Mixing Induced by an Electrokinetic Instability





Two 10 mM HEPES buffered solution. Bottom fluid has conductivity of 5 µS/cm.

Top fluid has Potassium chloride, conductivity of 50 µS/cm

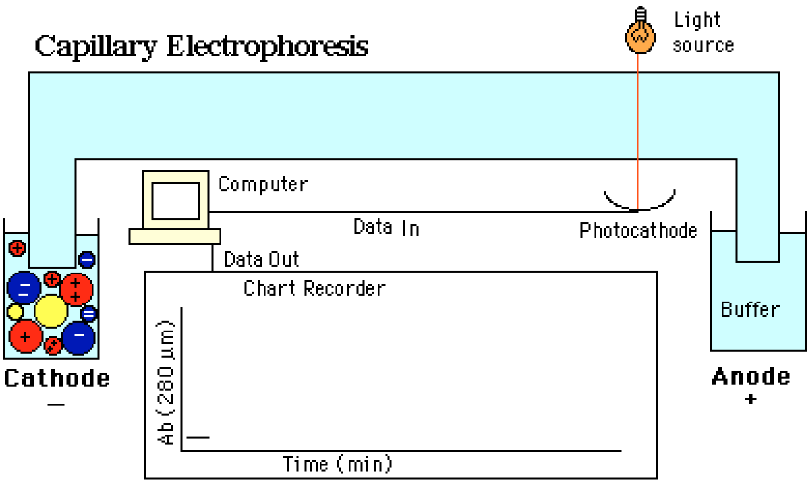
Courtesy of J. Santiago

Electrophoresis

Motion of charged surface relative to the stationary liquid by an applied electric field.

- Moving boundary electrophoresis: Solution containing positively and negatively charged particles are subjected to electric fields, and the particles move towards the oppositely charged electrode. This results in motion of the solution boundary, which is detected using Schleiren optical techniques.
- Steady state electrophoresis is obtained, when the positions of separated components do not change in time. This is commonly observed in isoelectric focusing (IEF) applications.
- Zone electrophoresis is the motion of ions across a concentration boundary that separates regions of high and low field strengths. It utilize a supporting medium to hold the sample, while an external electric potential is applied at the end of the supporting media.

Capillary Electrophoresis



Capillary Electrophoresis & Capillary Electrochromatography: http://www.ceandcec.com/cetheory.htm

A Simplified Electrophoretic Transport Model

$$\frac{\partial c_i}{\partial t} + \nabla \cdot \left(c_i \vec{u} + c_i \vec{v}_{ep,i} \right) = D \nabla^2 c_i$$

Species conservation for i[th] spec.

Convection — EP transport — Diffusion

$$\vec{v}_{ep} = \mu_{ep} \vec{E} \qquad \mu_{ep} = \frac{2\zeta\varepsilon}{3\eta}$$

Mobility is an empirical concept

$$\rho_f \left(\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} \right) = -\nabla P + \mu \nabla^2 \vec{u}$$

Fluid Flow→NS w/o f_{EK}

$$u_{eo} = -\frac{\zeta\varepsilon}{\eta} \vec{E}$$

HS Slip BC

Applied electric field

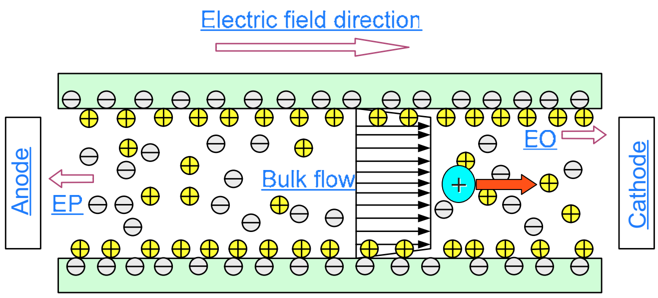
$$\vec{E} = -\nabla \phi, \quad \nabla^2 \phi = 0$$

Ermakov et al, **Analytic Chemistry**, 1998

Electrophoresis

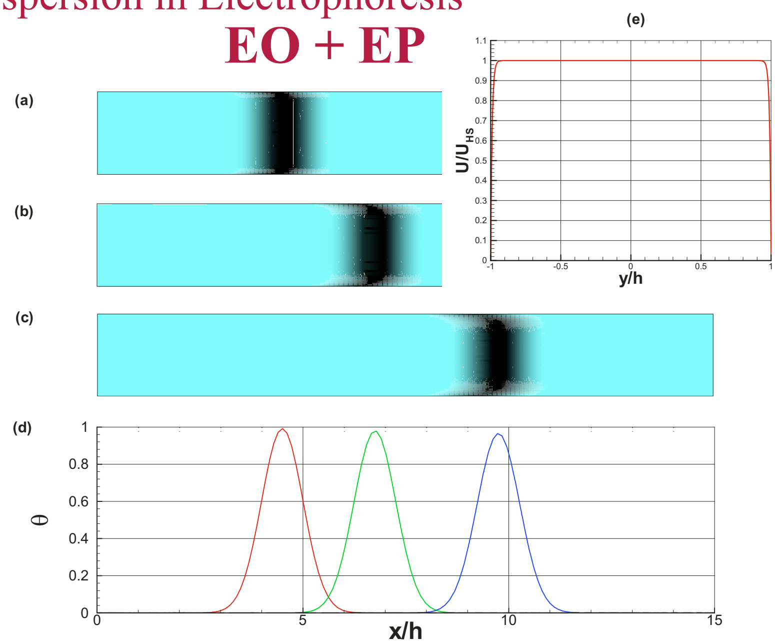
If $\zeta>0$ on the particle surface, then the particle will move towards the cathode.

This is known as ELECTROPHORESIS.

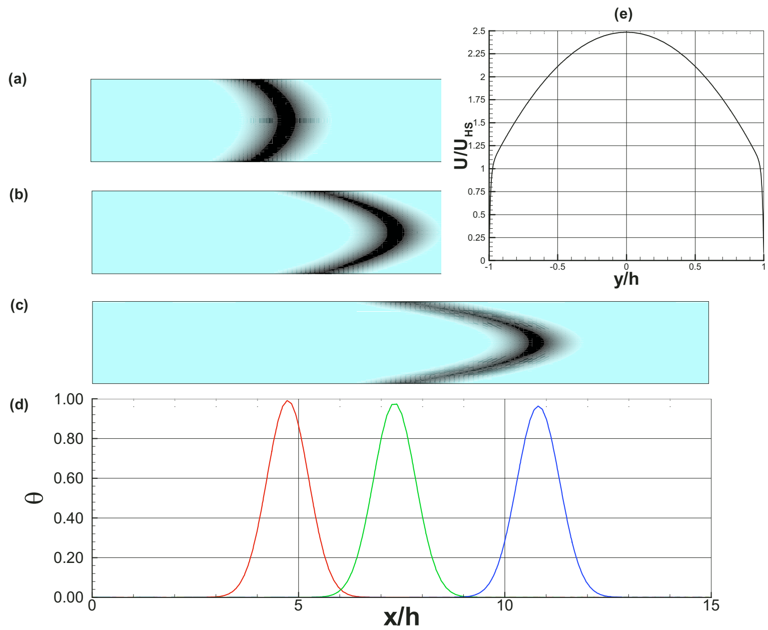


Dispersion in Electrophoresis

EO + EP



Dispersion in Mixed EO + EP + PD Flow



Taylor Dispersion

Channel averaged convective/diffusive transport results in dispersion with enhanced diffusion coefficient D_e

$$\frac{\partial \bar{n}}{\partial t} + U\frac{\partial \bar{n}}{\partial x} = D_e \frac{\partial^2 \bar{n}}{\partial x^2},$$

$$D_e = D\left(1 + \frac{Pe^2}{48}\right).$$

Poiseuille Flow
"Taylor-Aris"

$$D_e = D(1 + \alpha_o Pe^2),$$

$$\frac{4}{\alpha_o} \simeq 192 + \frac{4}{(\lambda_D^*)^{3/2}} + \frac{8}{(\lambda_D^*)^2},$$

EO Flow
$\lambda_D^* = \lambda/h$

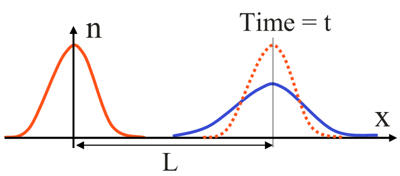
(Griffiths and Nelson, 1999)

For initial Gaussian distribution:

$$\bar{n}(x,0) = \frac{\bar{n}_o}{\sigma_o\sqrt{2\pi}} \exp\left(-\frac{x^2}{2\sigma_o^2}\right).$$

$$\bar{n}(x,t) = \frac{\bar{n}_o}{\bar{\sigma}\sqrt{2\pi}} \exp\left(-\frac{(x-Ut)^2}{2\bar{\sigma}^2}\right),$$

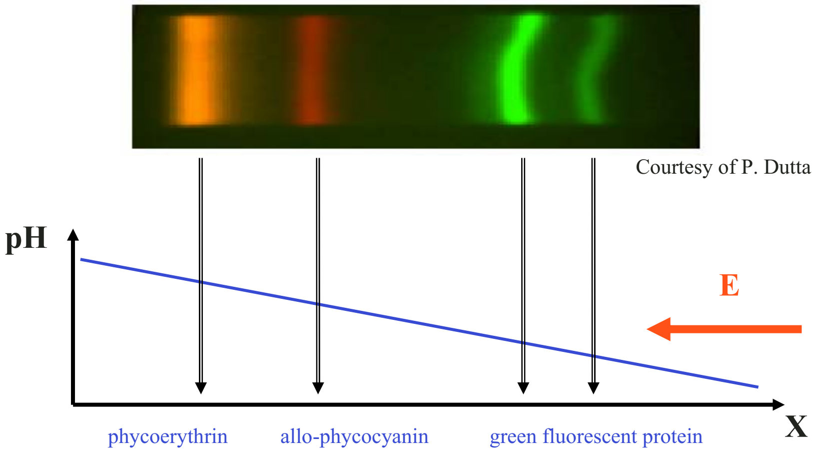
$$\bar{\sigma}^2 = \sigma_o^2 + 2tD_e$$



Migration Velocity V = L/t

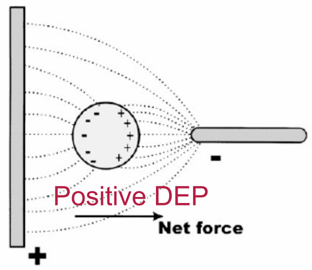
Iso-electric Focusing

IOF is the migration of charged particles under pH gradients to a location in the buffer, where they have zero net charge *(iso-electric point)* → EP transport under pH gradients

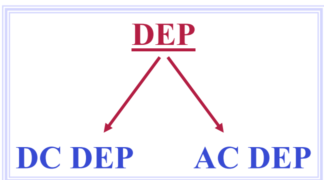


Dielectrophoresis

Motion of polarizable particles that are suspended in an electrolyte and subjected to a spatially non-uniform electric field.



Hughes, *Nanotechnology* **11** (2000)



Positive DEP: Particles that are more polarizable than the medium. Due to the inhomogeneous electric field, force is greater in the side facing the point. Hence, there is net motion towards the point electrode.

NegativeDEP: Particles are less polarizable than the surrounding medium. The dipole aligns counter to the field. Hence the particle is repelled from the high-field regions.

(AC) DEP: Time Averaged DEP Force

$$\vec{F}_{DEP} = 2\pi r^3 \varepsilon_m \operatorname{Re}\{k(\omega)\} \nabla \|E_{rms}\|^2$$

ε_m Permittivity of the medium

ε_p Permittivity of the particle

k(ω) Clausius-Mossoti factor $k(\omega) = \frac{(\varepsilon_p^* - \varepsilon_m^*)}{(\varepsilon_p^* + 2\varepsilon_m^*)}$

r particle radius

ε^* Complex permittivity $\varepsilon^* = \varepsilon - \sqrt{-1}\frac{\sigma}{\omega}$

σ conductivity

ω electric field frequency

Positive DEP, Re{k(ω)}> 0
Negative DEP, Re{k(ω)}< 0

***Insensitive* to Field Direction**

(AC) DEP for Particle Velocity

Eqn of Motion for suspended particle $m_p \frac{d\vec{V}}{dt} = \vec{F}_{DEP} - \vec{F}_{Drag}$

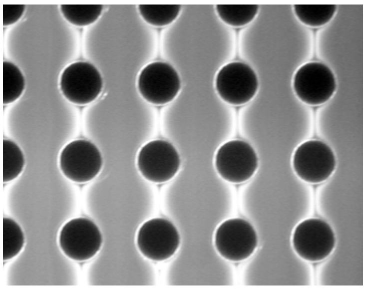
Assuming Stokes Drag (for a Sphere): $\vec{F}_{Drag} = 6\pi\mu r\vec{V}$

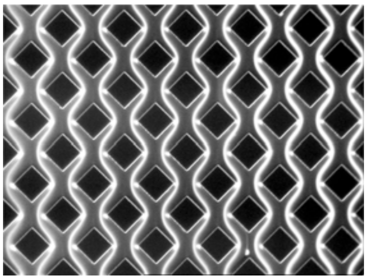
Neglecting Brownian Motion & Buoyancy Force and
Assuming Steady State:

$$\vec{V} = \frac{r^2 \varepsilon_m \operatorname{Re}[k(\omega)] \nabla \|E_{rms}\|^2}{3\mu}$$

- **DEP Velocity is proportional to the surface area of the particle**
- **DEP can be maintained either by DC or AC Electric fields**
- **DEP trapping is *reversible*.**

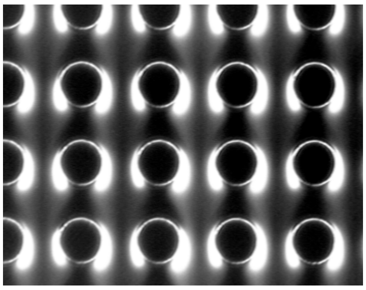
DC-DEP Example





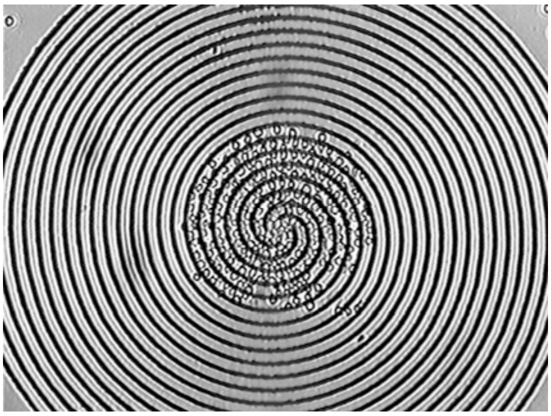
Filamentary Dielectrophoresis

Trapping Dielectrophoresis



Courtesy of E. Cummings,
Sandia National Laboratories

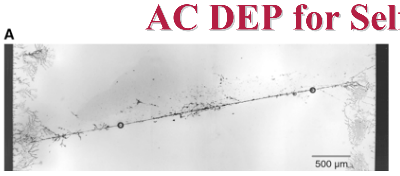
AC-DEP Example



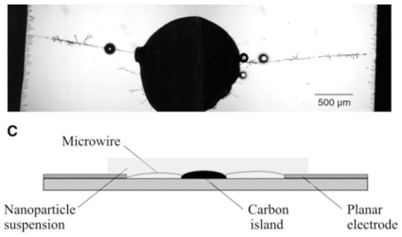
At 50 kHz, AC electric field polarize human leukemia cells, and moves them towards the center of four spiral electrodes

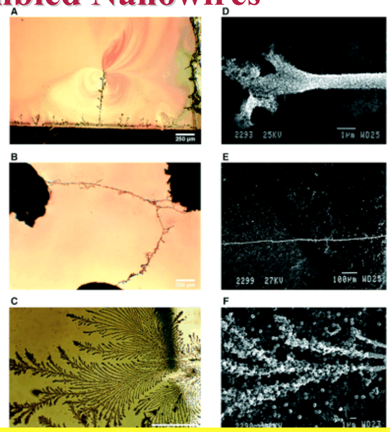
Courtesy of P. Gascoyne, UT MD Anderson

AC DEP for Self Assembled Nanowires



15 to 30*nm* diameter gold particles





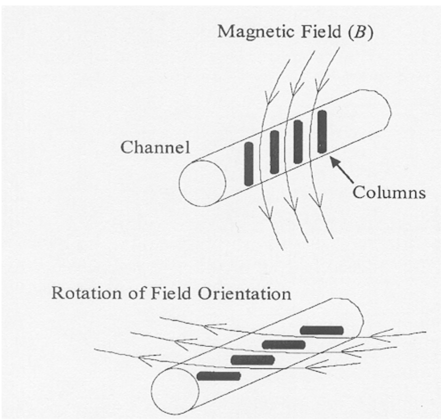
Hermanson, et al., **Science**, 294:1082–1086, 2001.

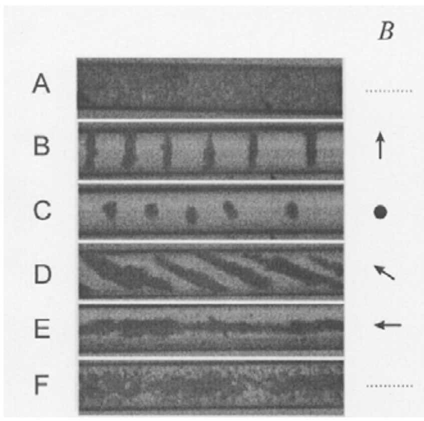
- Wire growth 50 µm/s with length ~ 5mm
- 50 to 200*V*, at 50 ~ 200*Hz*.
- Automatically form electrical connections to conductive islands or particles
- Self assembly & self repairing
- Promising for wet electronic and bio-electronic circuits

Courtesy of O. Velev

Other Particle Control Techniques: Magnetic Fields

Active Control of Supra-Particle Structures in Micro Channels





Hayes et al. *Langmuir* (2001)

Chaotically Stirred Micro Fluidic Systems

Ali Beskok

Associate Professor
Bio Micro Fluidics Laboratory
Mechanical Engineering Department
Texas A&M University
&

Mr. Ho-Jun Kim

Ph.D. Student

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Species Transport in Micro Scales

Despite low Reynolds numbers (Re ≈ 0.01)
Large particles and bio-molecules have very small mass diffusivities
⟶ large Schmidt numbers and large Peclet numbers

$$D = \frac{k_b T}{6\pi\pi\mu} \qquad Sc = \frac{\nu}{D} \qquad Pe = \frac{UL}{D} \qquad \frac{\text{Diffusion time } (L^2/D)}{\text{Convection time } (L/U)}$$

$$\frac{\partial C}{\partial t} + \vec{U} \cdot \nabla C = \frac{1}{Pe} \nabla^2 C$$

$Pe \propto 10^3 \sim 10^5$

Physical Parameters for large Bio-Molecules

Diffusing Particle in water	Diffusion coefficient (m^2/s)
Red Blood Cell	6.8×10^{-14}
Hemoglobin	7.3×10^{-11}

$\nu_{water} \approx 1.0\times10^{-6}$ m²/s

Need for Mixing Enhancement in Micro-Scales

- Lack of turbulence results in long time and/or length scales for diffusive mixing.

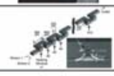
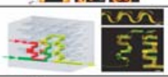
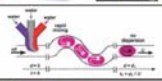
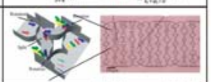
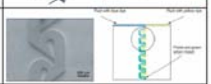
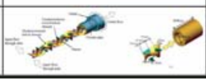
$$D = \frac{k_b T}{6\pi\pi\mu} \qquad Pe = \frac{UL}{D} \qquad \mathbf{Pe \propto 10^3 \sim 10^5}$$

For proteins in aqueous buffer with $D=10^{-10} m^2/s$, U=1cm/s, h=100μm ($Pe=10^4$) requires mixing length of L=100 cm.

Hence Mixing length $\propto Pe$

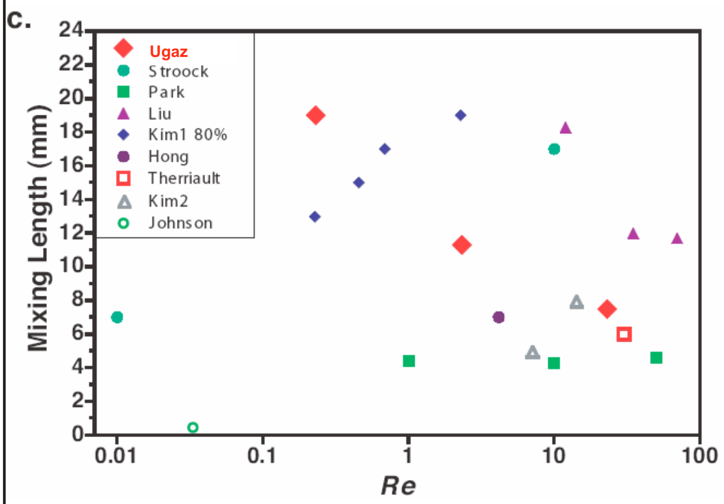
Chaotic stirring reduces the mixing time/length $\propto \ln Pe$

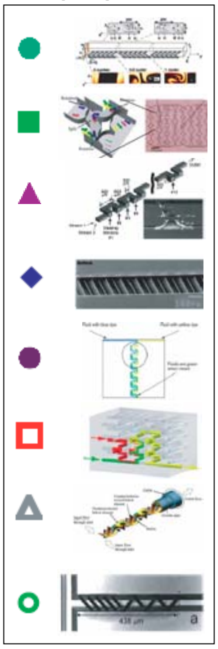
Requires *non-integrable* particle paths:
2-D Unsteady Flow, 3-D Steady or Unsteady Flow

Reference	*Re*	Mixing Length/Method	Effectiveness	Device Schematic
Bessoth et al., *Anal. Commun.* **1999**, 36, 213-215.	0.5 – 31	95% in 15 ms Fluorescence quenching	$0.5 \le Re \le 31$ Better at slow flow rates	
Liu et al., *J. Microelctromech. Sys.* **2000**, 9, 190-197.	6 – 70	>90% in ~ 11.7 mm[a] (*Re*=70) Normalized intensity	$Re > 35$ Better at high flow rates	
Johnson et al., *Anal. Chem.* **2002**, 74, 45-51.	0.03 – 0.45	>90% in 0.443 mm (*Re*~0.033) Normalized intensity	Better at slow flow rates	
Stroock et al., *Science* **2002**, 295, 647-651.	$10^{-2} – 10$	90% in 7 mm ($Re=10^{-2}$) σ of intensity distribution	$10^{-2} \le Re \le 10$ Better at slow flow rates	
Therrialut et al., *Nature Materials* **2003**, 2, 265-271.	0.7 – 70	90% in 6 mm (*Re*=30) Normalized intensity	$Re > 10$ Better at high flow rates	
Song et al., *Angew. Chem. Int. Ed.* **2003**, 42, 768-772.	0.28 – 8.4[b]	90% in 1.75 ms (*Re*=8.4) Normalized intensity	$5.3 \le Re \le 8.4$ Better at high flow rates	
Park et al., *J. Micromech. Microeng.* **2004**, 14, 6-14.	1 – 50	85% in 4 mm (*Re*=10) σ of intensity distribution	$1 < Re < 50$ Best at $Re = 10$	
Hong et al., *Lab Chip* **2004**, 4, 109-113.	0.08 – 8.31[b]	90% in 7 mm (*Re*=4.16)[b] Color intensity	$4 < Re < 8.3$[b] Better at high flow rates	
Kim et al., *J. Micromech. Microeng.* **2004**, 14, 798-805.	0.2 – 2.28	80% in 13 mm (*Re*=0.2) Normalized intensity	$0.2 < Re < 2.28$ Better at slow flow rates	
Kim et al., *J. Micromech. Microeng.* **2004**, 14, 1294-1301.	7 – 28	90% in 5 mm (*Re*=7) Normalized intensity	$7 < Re < 28$ Better at slow flow rates	

Courtesy of V. Ugaz, TAMU

Comparison of Various Mixers





Data points indicate mixing length to achieve 90% mixing except for the blue diamonds (80% mixing)

Courtesy of V. Ugaz

Objectives

- Enhancement of stirring using chaotic advection.
- Develop quantification tools for chaotic strength & mixing efficiency
  - Particle dispersion
  - Poincaré section
  - Finite Time Lyapunov Exponent
  - Mixing Index using species transport equations