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INTRODUCTION TO MICROFLUIDICS

8 - 26 August 2005

Part A - Electrokinetic Flow

Topic 1: Governing Equations of Pressure and Electrokinetic Flow

Topic 2: Analysis of the Governing Equations

Topic 3: Special Cases and Some Case Studies

J. MacINNES
University of Sheffield, U.K.



Part A. Electrokinetic Flow

Part B. Microreactors

Jordan MacInnes
Chemical and Process Engineering
University of Sheffield

ICTP Summer School
Introduction to Microfluidics
Trieste, Italy
August 8-26, 2005

Outline of lectures

Part A. Electrokinetic flow

- Topic 1. Governing equations of pressure and electrokinetic flow
- Topic 2. Analysis of the governing equations
- Topic 3. Special cases and some case studies

Part B. Microreactors

- Topic 4. Chemical reaction and microdevices
- Topic 5. The mixing problem
- Topic 6. Reaction case studies



Topic 1: Governing Equations of Pressure and Electrokinetic Flow

Jordan MacInnes
Chemical and Process Engineering
University of Sheffield

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Overview

- Introduction
- Governing equations
 - Flow equations
 - Electric field and charge
 - Species
 - Electric current and conductivity
 - Heat transfer
 - Chemical reaction
- Electric double layer and wall boundary conditions
- Electrokinetic effects, dielectrophoresis

Introduction

We will develop a computational methodology for flow processes in complex microfluidic devices.

- Flow processes include heat transfer, chemical reaction, electrokinetic effects, etc. (multiphase flow will not be considered and, generally, restriction will be to liquids)
- Microfluidic devices can have arbitrary geometry, involve time-dependent processes occurring over a large range of scales
- A compelling fact of microfluidic devices would appear to be that processes at scales of interest are predictable

Objective and Strategy

We aim to design devices computationally.

Must combine several strands of work:

- Theoretical modelling
- Numerical solution methodology
- Device fabrication
- Experimental methodology

Pressure flow – Electric flow

Two ways of moving liquids through microdevices are in use: imposing a pressure gradient and imposing an electric field.

Here, the general equations for electric flow are developed – pressure flow being just a special case of electric flow.

Each flow type has an important role to play.

It may be useful to state that:

- *Pressure flows are difficult to produce but easy to compute*
- *Electric flows are easy to produce but difficult to compute*

Governing equations

Let us consider, one by one, the continuum equations that must be satisfied.

Each may be derived by analysis of a physical law for an infinitesimal volume around an arbitrary point in space.

To describe the flow of reacting liquid with heat transfer and subjected to an electric field, we must consider:

- Conservation of mass
- Newton's second law
- Species transport
- First law of thermodynamics
- Gauss' law for electric field

Flow equations

The continuity equation enforces mass conservation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

Newton's second law relates fluid motion to the forces exerted.

For a Newtonian fluid:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] \right) + F_i$$

In words: fluid acceleration = pressure force + viscous force + other forces

Non-dimensional form of the flow equations

The importance of individual terms can be assessed by normalising variables so that the equation becomes non-dimensional and with new non-dimensional parameters arising.

Characteristic scales in the normalisations:

×	R	$\mu u_s / R$	μ	ρ	τ
(velocity)	(length)	(pressure)	(viscosity)	(density)	(time scale)

No parameters enter in the normalised continuity equation. For uniform density, the momentum equation becomes:

$$\left(\frac{\rho R^2}{\mu \tau} \right) \frac{\partial \rho u_i}{\partial t} + \text{Re} \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial^2 u_i}{\partial x_j^2}$$

Significance of the non-dimensional parameters

(1) Reynolds number:
$$\text{Re} = \frac{\rho u_s R}{\mu}$$

We see that for $\text{Re} \rightarrow 0$, the fluid acceleration associated with spatial variations in velocity may be neglected. This will often be the case in microfluidic applications.

(2) Non-dimensional time:
$$\frac{\mu \tau}{\rho R^2}$$

When periodic external forcing plays a significant role, τ will be the imposed period of the cycle and this is a second, independent parameter.

With no forcing, defines characteristic transient time:
$$\tau = \frac{\rho R^2}{\mu}$$

Electric field and charge

Electric field produced by a given distribution of charge in space can be expressed in terms of an electric potential as:

$$E_i = -\frac{\partial \phi}{\partial x_i}$$

The force per unit volume is given in terms of charge per volume by

$$F_i = \rho_e E_i$$

Electric potential (and electric field) is determined, for a given charge distribution by Gauss' law

$$\frac{\partial}{\partial x_j} \left(\epsilon \frac{\partial \phi}{\partial x_j} \right) = -\rho_e$$

where charge density is given by

$$\rho_e = \sum_{k=1}^N \rho e_k Y_k$$

Species transport

We must solve equations for species concentrations when non-uniform species concentration is significant or is of interest (e.g. chemical mixing, chemical reaction, electrokinetic flow).

Using mass fraction, Y_k as the concentration variable, the equation for species k is

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = -R_k + \frac{\partial}{\partial x_j} \left(\rho D_k \frac{\partial Y_k}{\partial x_j} + \rho Y_k \omega_k z_k F \frac{\partial \phi}{\partial x_j} \right)$$

In words: Change results from reaction + diffusion + electric migration

D_k is diffusivity, z_k is charge number, F is the Faraday constant

ω_k is electric mobility (related approximately to diffusivity by $\omega_k \Rightarrow \frac{D_k}{RT}$)

Parameters arising in species equation

(1) Transient time: $\tau = Sc \frac{\rho R^2}{\mu}$ where $Sc = \frac{\mu}{\rho D}$

(2) Peclet number (convection term): $Pe = Sc Re$

The Schmidt number large in liquids (1000 for aqueous solutions) so convection terms may not usually be dropped.

(3) Damkohler number (reaction term): $Da = \frac{R_o R^2}{\rho D Y}$

Relative importance of kinetic rate and diffusion rate.

(4) Electric migration terms: $\frac{z_o F \Delta \Phi}{RT}$

Depends on magnitude of imposed electric potential difference, $\Delta \Phi$

Electric current and conductivity

Charge conduction in a liquid is by movement of charged species. Thus, the species equations already presented govern electric current.

$$\frac{\partial \rho_e}{\partial t} + \frac{\partial i_j}{\partial x_j} = 0$$

may be derived from the species equation, where, for equal species diffusivities the current flux can be written:

$$i_j = -D \frac{\partial \rho_e}{\partial x_j} - \sigma \frac{\partial \phi}{\partial x_j} + \rho_e u_j \quad \text{where} \quad \sigma = \rho \sum_{k=1}^N Y_k \frac{z_k^2 F^2 \omega_k}{M_k}$$

This reduces to Ohm's law, $i_j = \sigma E_j$ only when the liquid is charge neutral.

Heat transfer

When heat transfer is important, we must solve the energy equation,

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} = \sum_{k=1}^N R_k \Delta h_k + \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) + \sigma \left(\frac{\partial \phi}{\partial x_j} \right)^2$$

The first term on the right hand side is energy of reaction and the final term is heat generation by Ohmic heating. Each term produces a New non-dimensional parameter.

Again, the convection terms produce a Peclet number $Pe_h = Pr Re$ based on thermal diffusivity.

Including heat transfer is relatively straightforward theoretically, although boundary conditions are usually only known at a distance from the flow domain.

Further equations

Chemical reaction can be expressed in terms of the rates of creation due to each of M reactions involved. For species k

$$R_k = \sum_{r=1}^M R_{rk}$$

where the reaction rate due to reaction r can be expressed in terms of concentrations, temperatures and stoichiometry using appropriate rate expressions.

Thermodynamic relations are also needed to allow enthalpy to be linked to temperature.

Boundary conditions

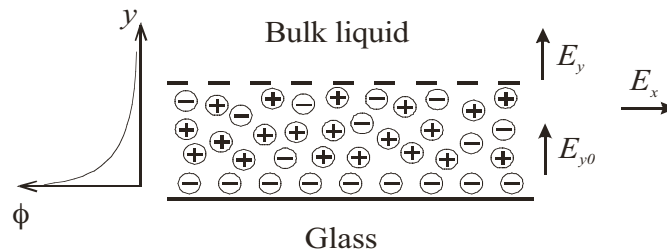
The usual boundary conditions for fluid flow computation can be used to complete the mathematical problem of determining the velocity, pressure, composition, temperature and electric field in a domain of interest.

Electrokinetic flow

In the case of the electric field equation (Gauss' law), one can show that for flow passages constructed of electrically insulating material, the normal gradient of electric potential is proportional to the wall charge per unit area. This relation provides the boundary condition for electric potential with the wall charge determined by surface thermodynamic equilibrium.

Electrical double layer

Double layer in liquid adjacent to a solid wall:



- Liquid and solid take on opposite charge
- For electrolyte liquid (containing ion species) charge is distributed out into the liquid adjacent to the wall
- Diffusion of ions normal to the wall is in balance with electric migration produced by the electric field due to the charge
- Double layer is typically several nm thick

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Electrokinetic flow

The two effects associated with application of an external electric field.

Electroosmosis

- External electric field exerts force on charged double layer liquid
- Motion transmitted to bulk liquid by shear stress

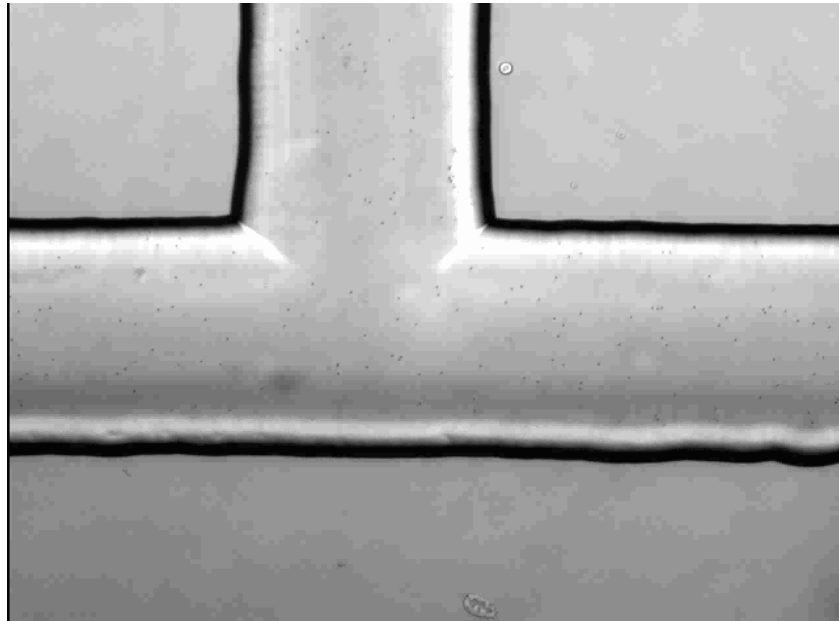
Electrophoresis

- External electric field produces electric migration of ion species
- Relative motion of species results from differences in mobility and charge number (electrophoretic separation)

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KCl solution with 1 μm latex particles



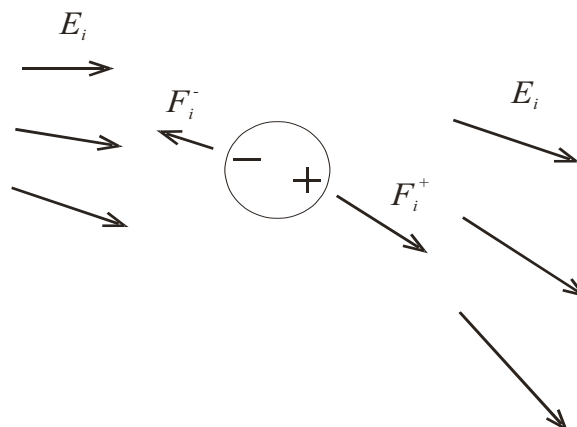
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A further electrical effect

Dielectrophoresis

- This is a further electric force that can be taken advantage of in some conditions
- It is the result of net Coulomb force acting on the separated charge of a particle in a non-uniform electric field



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Dielectrophoretic force

The force is given by (Pohl, Dielectrophoresis, 1978):

$$F_{Di} = \frac{8\pi^2}{3} r_P^3 \epsilon_M \alpha \frac{\partial E_i^2}{\partial x_i}$$

r_P is the size of particle (could be a single molecule)

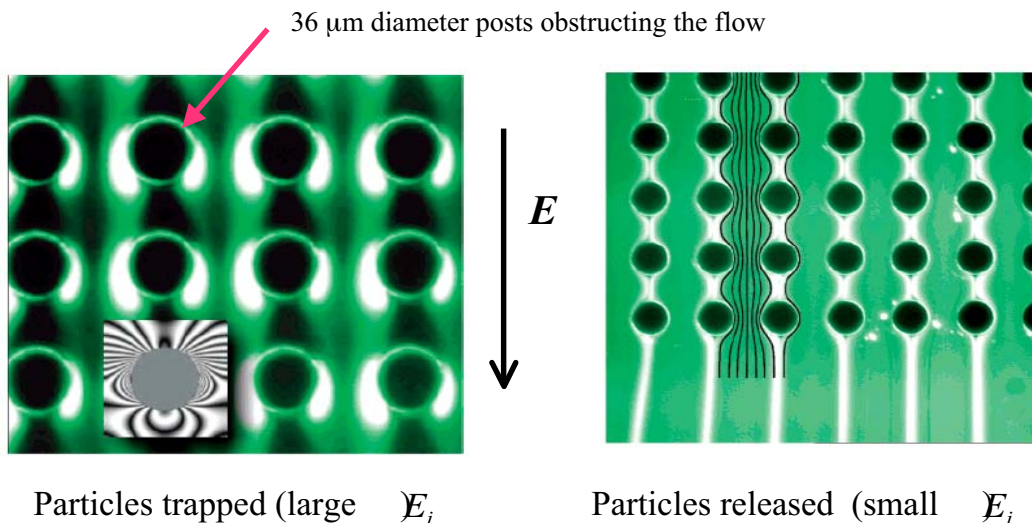
ϵ_M is the dielectric constant of the medium surrounding the particle

α is a function of the dielectric constants of the medium and the particle, approaches zero as the two dielectric constants become the same

Where the other electrokinetic effects move particles in the direction of E_i
 dielectrophoresis moves particles in the direction of $\partial E_i^2 / \partial x_j$

DC dielectrophoresis

Cummings and Singh (2003) show that geometric features to distort the electric field can be used to trap and release particles



(200 μm diameter latex particles tagged with fluorescent dye are used)

Scaling of dielectrophoresis

When is dielectrophoresis important?

Comparing this force to the level of force associated with inherent thermal energy,

$$F_T \approx k_B T / 2r_p$$

$$\frac{F_{Di}}{F_T} \propto r_p^4 \frac{\partial E_i^2}{\partial x_j}$$

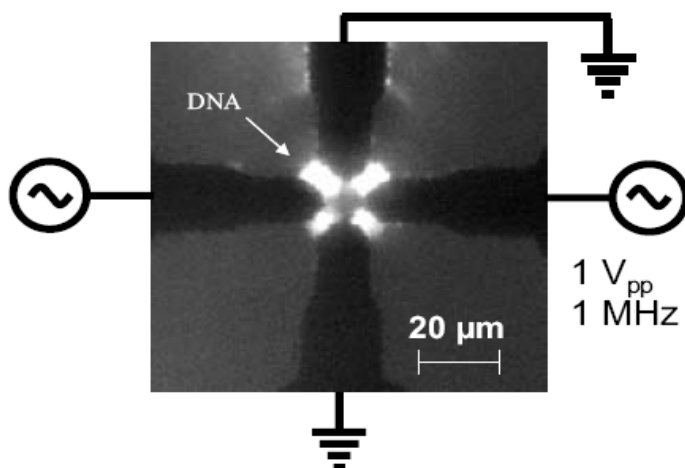
This suggests that for small particles such as molecules will not be significant in practice. But this is not the case!

Zheng et al. (2005), <http://nano.ece.uci.edu/papers/singlemolecule.pdf>

- Point out that the electric field simply needs to be made larger by moving the electrodes closer together to compensate for small r_p

DNA trapping

Zheng et al. also demonstrate experimentally the trapping of λ phage DNA using an electrode gap of 10 μm (shown below).



Electrodes with a 50 μm produced no effect on the DNA distribution even up to 10 V_{pp}.

Summary

We have introduced the general governing equations for Newtonian liquid flow in microdevice passages.

Thinness of the double layers (nanometers) in relation to typical flow passage size (micrometers) renders numerical solution of the full equations impractical.

Fortunately, accurate approximate representation of the double layer region is possible. The 'slip velocity' approximation is developed in Topic 2.

In Topic 3, useful special cases are considered and case studies are presented.



Topic 2. Analysis of the Governing Equations

Jordan MacInnes
Chemical and Process Engineering
University of Sheffield

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Overview

- Simple 1-D analytical solutions for double layer
 - Double layer with no flow
 - Developed flow between parallel walls
- Developed flow in channel of arbitrary section shape
- Order of magnitude analysis for double layer regions
- Electroneutrality in bulk flow regions
- ‘Slip velocity’ boundary treatment
- Time scales
- An example: reacting, uniform-property, alternating flow in a T-junction

Double layer adjacent to a planar wall (1)

No external field; uniform properties.
(Gouy-Chapman/Debye-Huckel solution)

Species equation: $D_k dY_k = -Y_k \omega_k z_k F d\phi$

$$\text{has solution } Y_k = Y_{kB} \exp\left\{-\frac{z_k F}{RT}(\phi - \phi_B)\right\} \quad (D_k = \omega_k RT)$$

$$\text{Gauss' law with } \psi = \phi - \phi_B : \quad \frac{d^2\psi}{dy^2} = -\frac{\rho F}{\epsilon} \sum_{k=1}^N \frac{z_k}{M_k} Y_{kB} \exp\left\{-\frac{z_k F \psi}{RT}\right\}$$

with B.C.'s $\psi = 0$ for $y \rightarrow \infty$, $\psi = \zeta$ at $y = 0$

Analytical solution difficult for all but simple electrolyte solutions.

Double layer adjacent to a planar wall (2)

Linearisation of the exponential in Gauss' law results in

$$\frac{d^2\psi}{dy^2} = \kappa^2 \psi$$

where κ is the Debye-Huckel parameter $\kappa = \sqrt{\frac{\rho F^2}{\epsilon RT} \sum_{k=1}^N \frac{z_k^2 Y_{kB}}{M_k}}$

$1/\kappa$ is the Debye length is a measure of double layer thickness.

Solution for electric potential in the double layer: $\psi = \zeta \exp(-\kappa y)$

The linearisation is accurate for $z_k F |\zeta| / RT < 2$ (Hunter, 2001).

($|\zeta| < 50$ mV for ions of unit charge and ambient temperature.)

Developed flow between parallel walls (1)

Species solution unchanged since no streamwise variation.

$$\begin{aligned} \text{With the new B.C.s} \quad \psi &= \zeta & \text{at } y &= 0 & \text{(lower wall)} \\ \partial\psi/\partial y &= 0 & \text{at } y &= h/2 & \text{(channel centre)} \end{aligned}$$

$$\text{Gauss' law gives} \quad \psi = \zeta \left\{ \frac{\exp(-\kappa y) + \exp(-\kappa h)\exp(\kappa y)}{1 + \exp(-\kappa h)} \right\}$$

$$x \text{ momentum reduces to} \quad 0 = -\frac{dp}{dx} - \varepsilon E_x \frac{d^2\psi}{dy^2} + \mu \frac{d^2u}{dy^2}$$

$$\text{With B.C.s} \quad u = 0 \quad \text{at } y = 0 \quad \text{and} \quad du/dy = 0 \quad \text{at } y = h/2 :$$

$$u = \frac{1}{\mu} \frac{dp}{dx} \left(\frac{y^2}{2} - \frac{hy}{2} \right) + \frac{\varepsilon E_x}{\mu} (\psi - \zeta)$$

Developed flow between parallel walls (2)

Let us examine the solution, non-dimensionalised using ζ and the 'slip' velocity scale appearing in the solution

$$u_s = -\frac{\varepsilon \zeta E_x}{\mu}$$

The result is

$$\begin{aligned} u^* &= \frac{1}{2} \beta (y^{*2} - y^*) - (\psi^* - 1) \\ \psi^* &= \frac{\exp(-\gamma y^*) + \exp(-\gamma)\exp(\gamma y^*)}{1 + \exp(-\gamma)} \end{aligned}$$

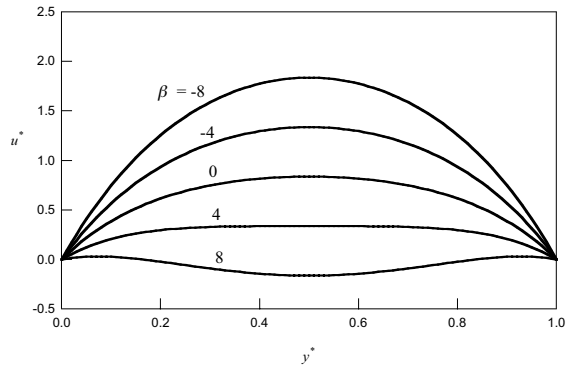
With the solution depending on the two parameters

$$\beta = \frac{h^2}{\mu u_s} \frac{dp}{dx} \quad \gamma = \kappa h$$

Developed flow between parallel walls (3)

Velocity profiles

$$\gamma = 5$$



Representative values for γ (0.1 mM KCl solution)

h	100 μm	10 μm	1 μm	0.1 μm
γ	3000	300	30	3

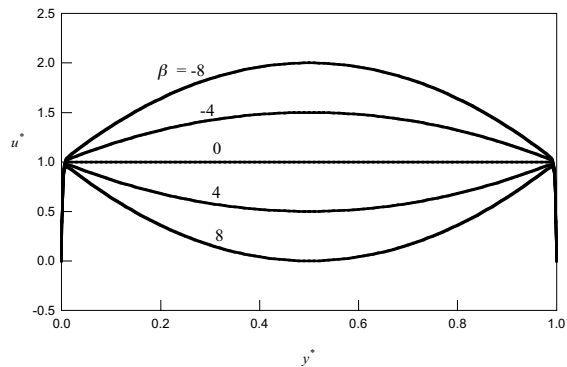
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Developed flow between parallel walls (4)

Velocity profiles

$$\gamma = 500$$



For $\gamma \rightarrow \infty$
solution becomes

$$u = \frac{1}{\mu} \frac{dp}{dx} \left(\frac{y^2}{2} - \frac{hy}{2} \right) + u_s$$

That is: the usual pressure flow solution + constant slip velocity

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Developed flow, arbitrary channel section

Thus, for $\gamma \rightarrow \infty$ one can ‘construct’ the electrokinetic developed flow velocity profile as the sum of the usual pressure flow profile and the constant slip velocity.

We will be interested later in the relation between flow rate and electric current and imposed pressure and potential gradient. Integration of the velocity profile produces

$$Q = -\frac{R^2 A}{f\mu} \frac{dp}{dx} + \frac{\varepsilon\zeta A}{\mu} \frac{d\phi}{dx} \qquad I = -\sigma A \frac{d\phi}{dx}$$

Where the ‘friction factor’, f , is determined by the developed flow pressure profile and is a function only of channel section shape.

Complex flow conditions

The preceding consideration of developed flow is not of great interest in tackling problems in actual microfluidic devices.

Perhaps not surprisingly, for thin double layer conditions, the behaviour in the double layer region is *locally* identical to that found in the preceding solutions, i.e. the use of a slip velocity in place of detailed solution within the double layer region is possible.

Cummings et al. 1999 and 2000, Mosher et al. 1992, Overbeek 1952 and Probstein 1994 have all shown that replacing the double layer by the slip velocity is accurate for small double layer thickness.

That work has been extended to cases with non-uniform species concentration, chemical reaction and heat transfer by MacInnes (2002).

Order of magnitude analysis (1)

One can establish the validity of the 1-D analytical result for the double layer using an order of magnitude analysis of the equations.

If each equation takes the same form as in the analytical solution, then the relation between bulk flow and the wall, point by point on the wall, remains valid: the slip velocity approach holds.

Characteristic scales:

- Length for tangential variation ξ and normal variation $1/\kappa$
- Velocity difference u_s
- External electric potential $\Delta\Phi$
- Species mass fraction γ
- Temperature difference Θ
- Reaction rate R

Order of magnitude analysis (2)

Applying these normalisations to the tangential momentum equation (velocity component u and x direction) and noting from continuity that normal velocity, v , must be order u_s/γ

$$\frac{\partial \rho u}{\partial t} + \frac{\partial \rho u u}{\partial x} + \frac{\partial \rho v u}{\partial y} + \frac{\partial \rho w u}{\partial z} =$$

$$O\left(\frac{\rho \xi^2}{\mu \tau}\right) \quad O(\text{Re}) \quad O(\text{Re}) \quad O(\text{Re})$$

$$-\frac{\partial p}{\partial x} + \varepsilon \frac{\partial^2 \phi}{\partial x^2} \frac{\partial \phi}{\partial x} + \varepsilon \frac{\partial^2 \phi}{\partial y^2} \frac{\partial \phi}{\partial x} + \varepsilon \frac{\partial^2 \phi}{\partial z^2} \frac{\partial \phi}{\partial x} + \mu \frac{\partial^2 u}{\partial x^2} + \mu \frac{\partial^2 u}{\partial y^2} + \mu \frac{\partial^2 u}{\partial z^2}$$

$$O(1) \quad O\left(\frac{\Delta\Phi}{\zeta}\right) \quad O(\gamma^2) \quad O\left(\frac{\Delta\Phi}{\zeta}\right) \quad O(1) \quad O(\gamma^2) \quad O(1)$$

where now $\gamma = \kappa \xi$

Conditions for slip velocity treatment

Momentum equation	$\gamma^2 \gg 1$	$\gamma^2 \gg \text{Re}$	$\gamma^2 \gg \frac{\Delta\Phi}{\xi}$
Species equations	$\gamma^2 \gg \text{ScRe}$	$\gamma^2 \gg \text{Da}$	
Energy equation	$\gamma^2 \gg \text{PrRe}$	$\gamma^2 \gg \text{Da} \frac{\text{Pr} Y \Delta h}{\text{Sc} C_p \Theta}$	
Gauss' law	$\gamma^2 \gg \frac{\Delta\Phi}{\xi}$		

Electroneutrality in the bulk flow

The assumption of charge neutrality in the bulk liquid is now justified. Order of magnitude analysis for bulk flow is used.

Ratio of net charge density to ion charge density $\frac{\rho_I}{\rho_e} = O\left(\frac{\Delta\Phi}{\gamma^2 \xi}\right)$

Thus, imbalance in ion charge is negligible under preceding conditions.

Charge transport equation reduces to $\frac{\partial}{\partial x_j} \left(\sigma \frac{\partial \phi}{\partial x_j} \right) = 0$

Combining with Gauss' law gives the charge density to be

$$\rho_e = \frac{\varepsilon}{\sigma} \frac{\partial \sigma}{\partial x_j} \frac{\partial \phi}{\partial x_j}$$

Slip velocity treatment

Collection of boundary conditions used in place of the double layer:

Velocity	$u_i = -\frac{\varepsilon\zeta E_i}{\mu}$
Electric potential	$n_i \frac{\partial \phi}{\partial x_i} = 0$
Species (no surface reaction)	$n_i \frac{\partial Y_k}{\partial x_i} = 0$
Temperature	$n_i \frac{\partial T}{\partial x_i} = \frac{q}{\lambda}$

Time-dependent flow (1)

The slip velocity breaks down when channel size becomes small,
 But also when the flow is forced (by alternating voltage or pressure)
 at high frequency. The inverse frequency must be large compared to
 the double layer time scales

	Momentum	Energy	Species
	$\tau = \frac{\rho}{\mu\kappa^2}$	$\tau = \frac{\rho C_P}{\lambda\kappa^2}$	$\tau = \frac{1}{D\kappa^2}$
0.1 mM KCl solution	1 ns	10 ns	1 μ s

Time-dependent flow (2)

Typical operation of electrokinetic microdevices using switching at intervals measured in seconds. The bulk flow time scales are

	Momentum	Energy	Species
	$\tau = \frac{\rho \xi^2}{\mu}$	$\tau = \frac{\rho C_p \xi^2}{\lambda}$	$\tau = \frac{\xi^2}{D}$
100 μm aqueous solution	10 ms	100 ms	10 s

Flow and temperature can be treated as quasi-steady. Species can not.

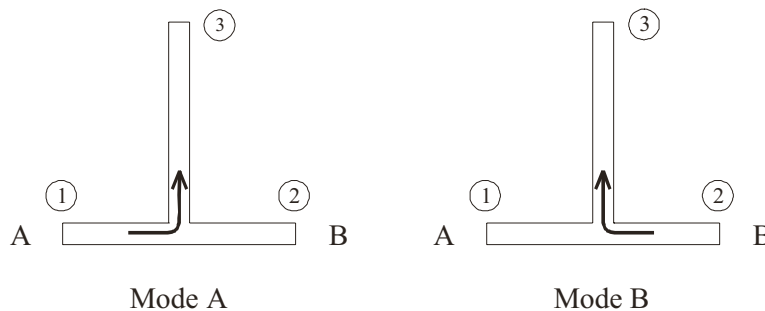
Example computation (1)

Reacting flow of uniform property liquid, alternating between two modes. Both pressure and electric flow considered.

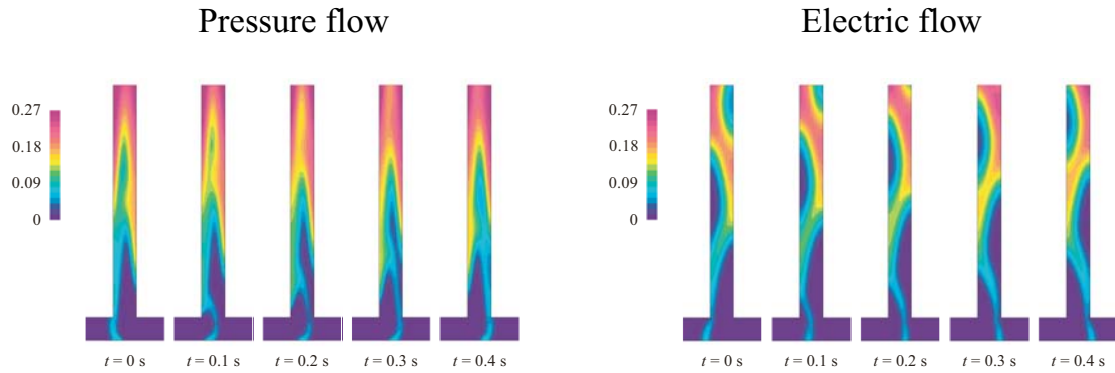
$$\text{Re} = 0.12$$

$$\text{Da} = 10$$

$$\text{Sc} = 1000$$

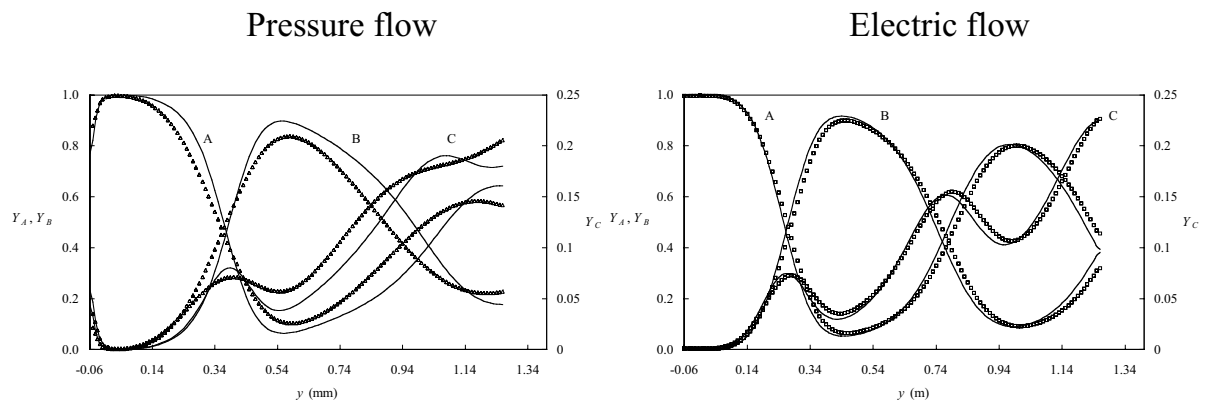


Example computation (2)



Plots of product concentration during injection of A.

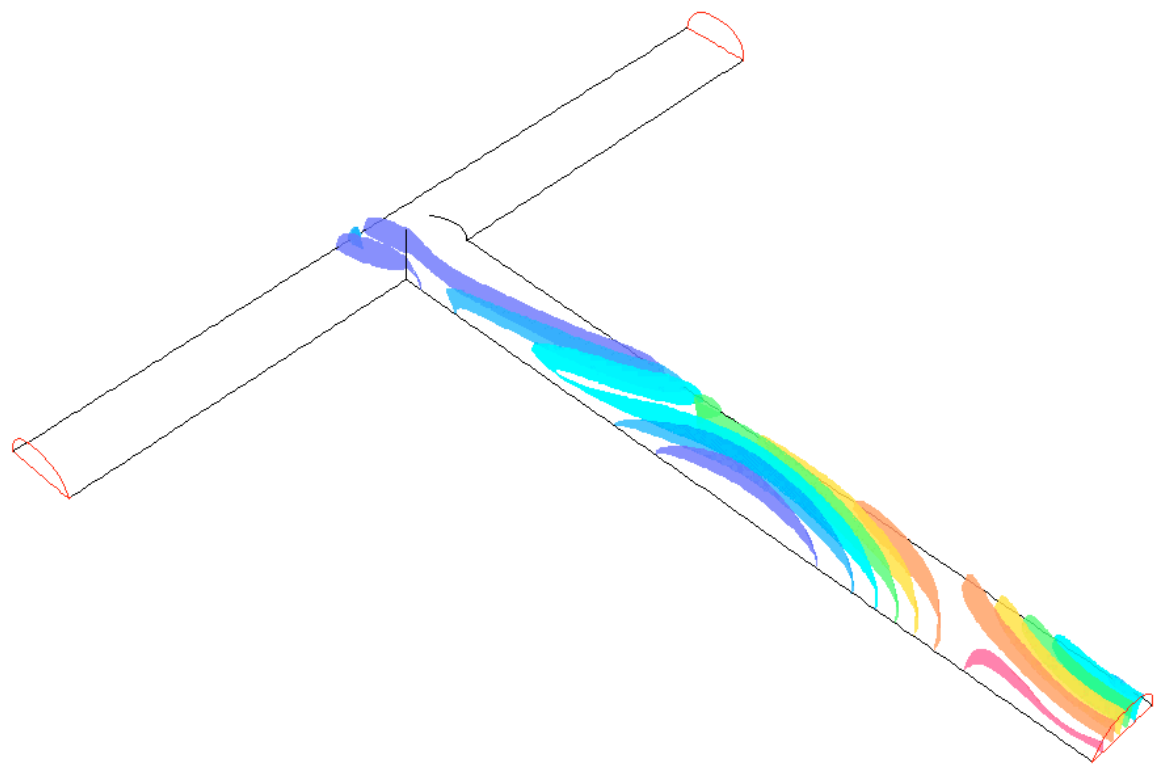
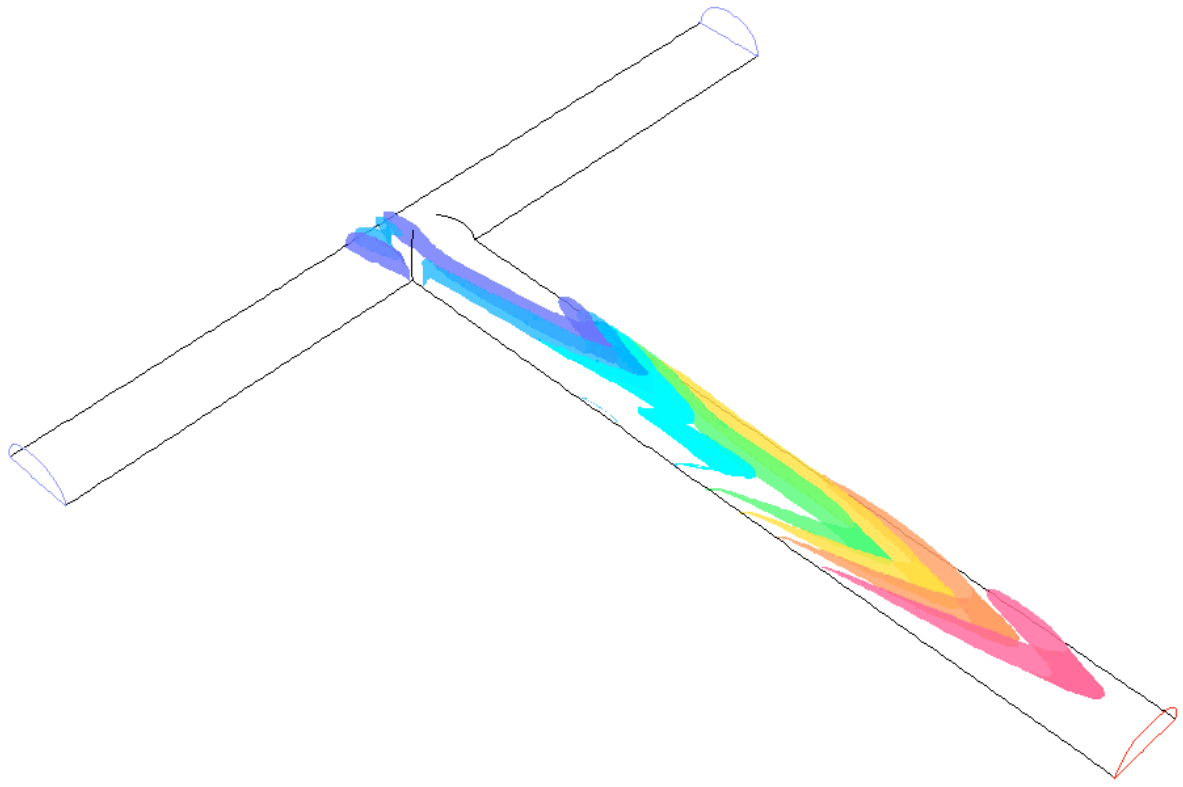
Example computation (3)



Plots of species concentrations along the main channel.

Curves - 2D computation

Symbols - 3D computation



Summary

Simple classical solutions for electric field and ion concentration have been presented to provide background for a general treatment.

The conditions under which the double layer can be represented by the classical one dimensional solution have been outlined.

The slip velocity treatment has been presented and the role of time scales considered.

An example problem has been presented.



Topic 3. Special Cases and Some Case Studies

Jordan MacInnes
Chemical and Process Engineering
University of Sheffield

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Overview

- Modelling levels
- Low Reynolds number
 - Network analysis
 - 'Linking' boundary conditions
- Ideal electrokinetic flow
- Case studies
 - Uniform property flow in a T-junction
 - A switching junction
 - Non-uniform property electrokinetic flow
- Summary

Modelling levels

Computing complex flows requires judicious use of different modelling levels.

1. *Full governing equations (2D and 3D)*
2. *Slip velocity treatment (2D and 3D)*
3. *Ideal electrokinetic flow (2D and 3D)*
4. *Network analysis (0D and 1D)*

The first two in the list were introduced in the previous lectures. The final two will now be presented.

Often, the most effective computational approach uses different levels of modelling for different parts of a microfluidic device.

The case of $Re \rightarrow 0$

The limit of small Reynolds number is potentially important.

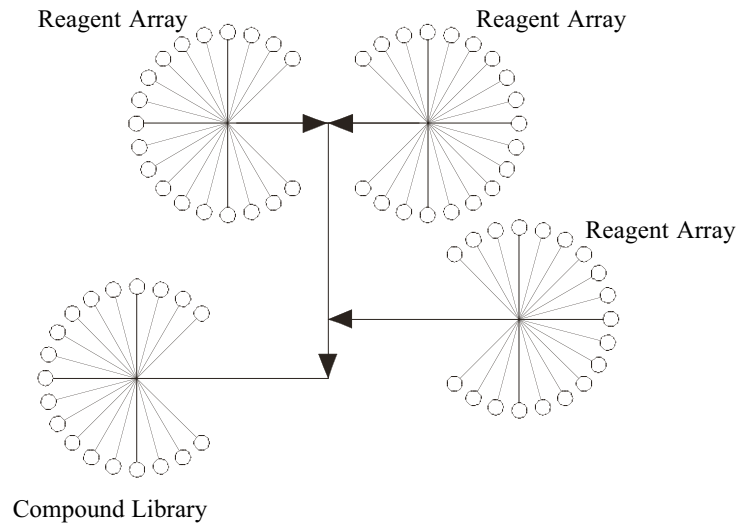
- Electrokinetic flows are nearly always at $Re < 0$.
- A likely direction in the development of microfluidic devices is towards smaller channel size.

Disturbance lengths near junctions and inlets become small and uniform channel sections can be treated as developed over the entire length to a good approximation.

For example, entry disturbance length for flow into a circular section Channel is

$$\frac{x_e}{d} \approx \frac{Re}{20} \quad \text{White (1999)}$$

A complex microfluidic network



Network analysis (1)

The standard methods used to analyse electric resistance circuits can be extended to treat microfluidic networks comprising interconnected uniform channel segments. (MacInnes et al., 2003)

In addition to Ohm's law for current flow, one has the developed flow relation between volume flow rate and pressure and potential differences:

$$I_i = -\sigma_i A_i \frac{\Delta\phi_i}{\Delta s_i} \qquad Q_i = -\frac{R_i^2 A_i}{f_i \mu_i} \frac{\Delta p_i}{\Delta s_i} + \frac{\varepsilon_i \zeta_i A_i}{\mu_i} \frac{\Delta\phi_i}{\Delta s_i}$$

Two continuity constraints apply:

1. At each junction charge and mass flow must balance
2. Pressure and potential must sum to zero around any loop

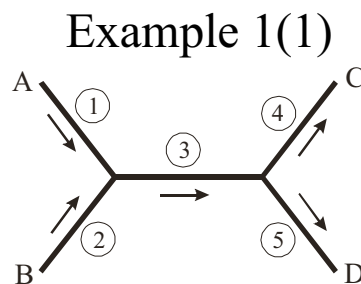
Network analysis (2)

Two types of problems will be encountered:

- 1) Conditions imposed at reservoirs are known and we wish to determine the resulting flow state
- 2) We wish to determine reservoir conditions needed to produce a given flow state

In the first type, the known reservoir differences are simply used in the loop constraints.

In the second, the loop constraints are replaced by constraints on flow rates in particular channel segments; the loop constraints become equations for determining the reservoir differences.

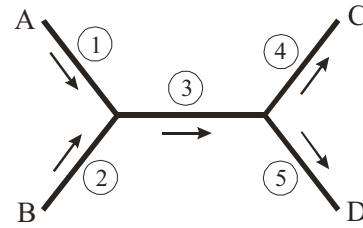


The arrows show the sign convention for positive flow direction and Positive pressure and potential differences.

We will work this problem for both imposed reservoir conditions and imposed flow state.

To simplify the algebra, each segment will taken as having the same section shape and the same length; properties will be the same in each segment.

Example 1(2)



Four junction balances:

$$Q_1 + Q_2 - Q_3 = 0 \quad \text{or} \quad -\alpha(\Delta p_1 + \Delta p_2 - \Delta p_3) + (\Delta\phi_1 + \Delta\phi_2 - \Delta\phi_3) = 0$$

$$Q_3 - Q_4 - Q_5 = 0 \quad \text{or} \quad -\alpha(\Delta p_3 - \Delta p_4 - \Delta p_5) + (\Delta\phi_3 - \Delta\phi_4 - \Delta\phi_5) = 0$$

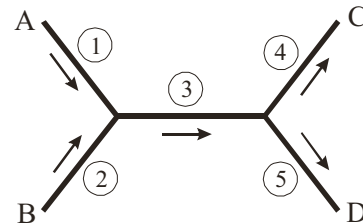
$$I_1 + I_2 - I_3 = 0 \quad \text{or} \quad (\Delta\phi_1 + \Delta\phi_2 - \Delta\phi_3) = 0$$

$$I_3 - I_4 - I_5 = 0 \quad \text{or} \quad (\Delta\phi_3 - \Delta\phi_4 - \Delta\phi_5) = 0 \quad \alpha = R^2 / f\varepsilon\zeta$$

Six independent loop equations:

$$\begin{aligned} \Delta p_1 + \Delta p_3 + \Delta p_4 &= p_C - p_A & \Delta p_2 + \Delta p_3 + \Delta p_4 &= p_C - p_B & -\Delta p_4 + \Delta p_5 &= p_D - p_C \\ \Delta\phi_1 + \Delta\phi_3 + \Delta\phi_4 &= \phi_C - \phi_A & \Delta\phi_2 + \Delta\phi_3 + \Delta\phi_4 &= \phi_C - \phi_B & -\Delta\phi_4 + \Delta\phi_5 &= \phi_D - \phi_C \end{aligned}$$

Example 1(3)



Now consider the second type of problem.

We will work out conditions for flow from A to D with no flow in 2 and 4. To make the problem interesting let us produce flow in segments 1 and 5 using just pressure difference, in segment 3 using just electric field.

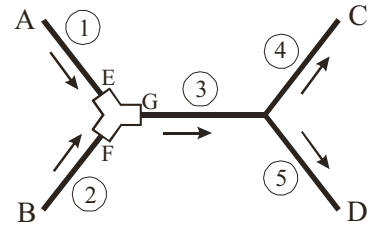
Junction balance as before.

Loop constraints are replaced by the direct flow constraints:

$$\begin{aligned} -\alpha\Delta p_1 &= Q^* & -\alpha\Delta p_3 &= 0 & -\alpha\Delta p_5 &= Q^* \\ \Delta\phi_1 &= 0 & \Delta\phi_3 &= Q^* & \Delta\phi_5 &= 0 \end{aligned}$$

where $Q^* = Q\mu\Delta s / \varepsilon\zeta A$

Example 2(1)



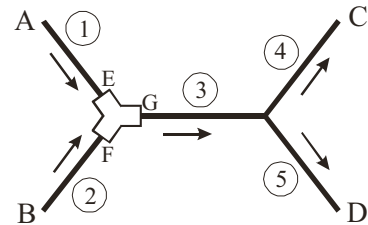
In this example, network analysis is used to arrive at boundary conditions at E, F and G for a detailed computation at one of the junctions. Reservoir conditions at A, B, C and D are known.

This is simply three network analyses, one for each of the networks connected to the flow boundaries of the computational domain.

Provided the flow boundaries are in the developed flow region away from the junction, we know that at each flow boundary pressure and electric potential are uniform.

The boundary values of pressure and potential can be related to reservoir values using straightforward application of the network analysis.

Example 2(2)



Resulting boundary conditions:

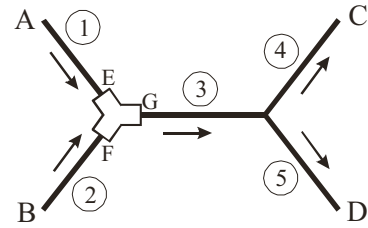
$$\text{At E: } \phi_E = \phi_A - \frac{dsI_E}{\sigma A} \quad p_E = p_A - \frac{fds_1(\sigma\mu Q_E + \varepsilon\zeta I_E)}{\sigma R^2 A}$$

$$\text{At F: } \phi_F = \phi_B - \frac{dsI_F}{\sigma A} \quad p_F = p_B - \frac{fds_2(\sigma\mu Q_F + \varepsilon\zeta I_F)}{\sigma R^2 A}$$

$$\text{At G: } \phi_G = \frac{I_G(ds_3 ds_4 + ds_3 ds_5 + ds_4 ds_5) + \sigma A(\phi_C ds_5 + \phi_D ds_4)}{\sigma A(ds_5 + ds_4)}$$

$$p_G = \frac{(\sigma f\mu Q_G + \varepsilon f\zeta I_G)(ds_3 ds_4 + ds_3 ds_5 + ds_4 ds_5) + \sigma R^2 A(p_C ds_5 + p_D ds_4)}{\sigma R^2 A(ds_5 + ds_4)}$$

Example 2(3)



The appearance of current and volume flow rates in the preceding relations couples these equations to the junction computation through integrations over the flow boundaries:

$$\begin{aligned}
 Q_E &= -\int_E u_i n_i dA & I_E &= \int_E \sigma \frac{\partial \phi}{\partial x_i} n_i dA \\
 Q_F &= -\int_F u_i n_i dA & I_F &= \int_F \sigma \frac{\partial \phi}{\partial x_i} n_i dA \\
 Q_G &= \int_G u_i n_i dA & I_G &= -\int_G \sigma \frac{\partial \phi}{\partial x_i} n_i dA
 \end{aligned}$$

Ideal electrokinetic flow

Cummings et al. (2000) show that for uniform property electrokinetic flow

$$u_i = aE_i$$

Where, clearly, to be consistent with the slip velocity boundary condition

$$a = -\varepsilon \zeta / \mu$$

Thus, the electric field and velocity field are related by a constant.

This state of similarity is violated for non-uniform properties as occurs when species concentration is non-uniform or wall coatings are employed.

Case Study 1(1)

Uniform property T-junction flow, MacInnes, et al., Phys. Fluids (2003)

Objective: Verification of flow equations, pressure & electric

Three cases: electric, pressure, mixed (all steady flows)

$Re = 0.04$, $\gamma = 10^4$, pH 8, 0.05 M KCl solution

Computations to within 2% uncertainty (Fluent 5)

Measurements of velocity to within 5% uncertainty (PTV)

Control of experimental conditions to within 1%

All characteristics needed for computation determined:

Network and channel geometry

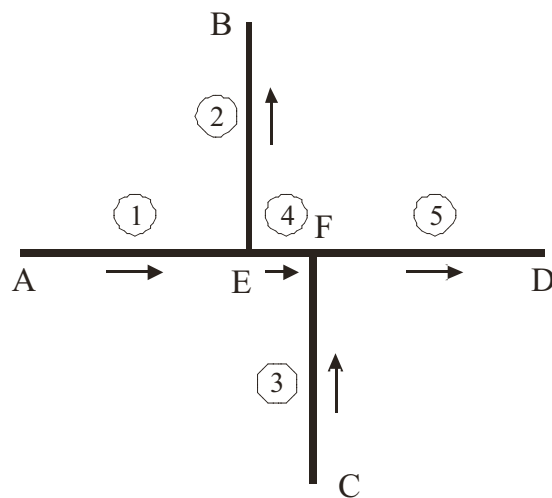
Liquid properties (viscosity, zeta potential)

Seed particle properties (electric mobility)

ICTP Microfluidics 2005, MacInnes

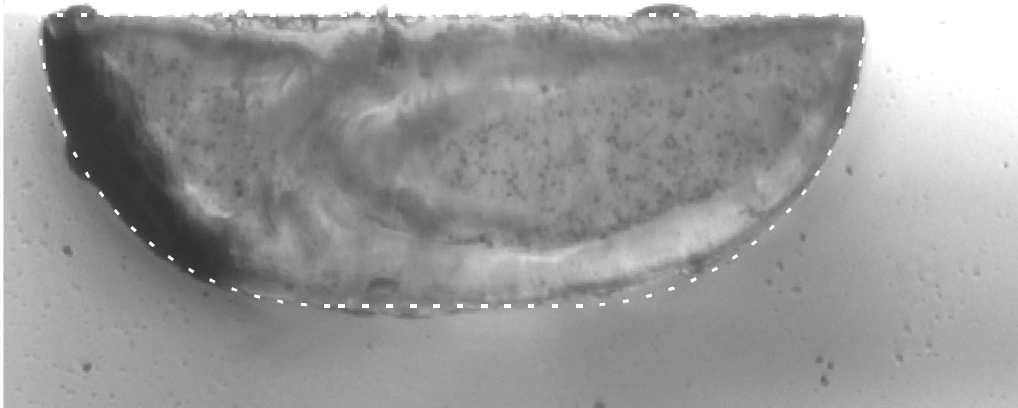
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Case Study 1(2)

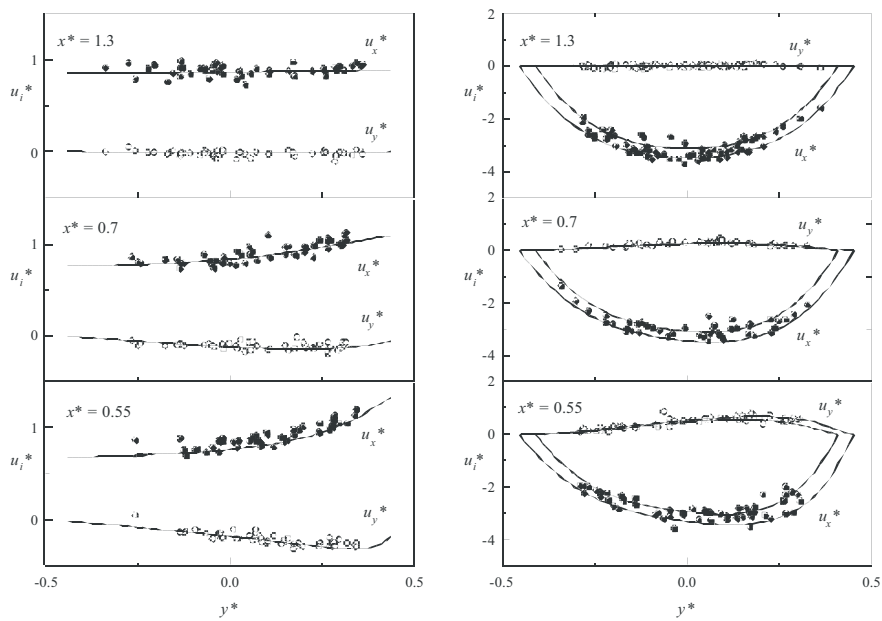


ICTP Microfluidics 2005, MacInnes

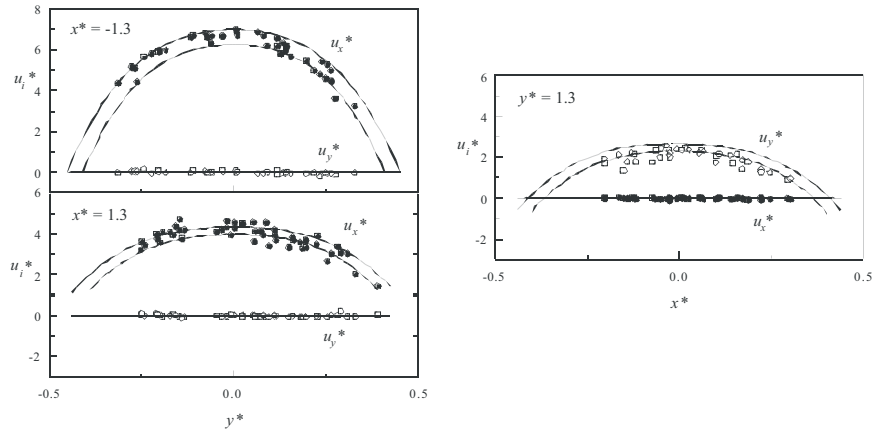
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Case Study 1(4)



Case Study 1(5)



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Case Study 2(1)

Switching junction, MacInnes, Trans. IChemE (2003)

Objective: change from injection of one liquid to another
with a sharp transition between the two

Applications: automated sample selection (combinatorial chemistry)
slug microreactor (Fletcher et al., 1999, 2000)

Time-dependent alternating flow, uniform liquid properties ($Re=0.01, Pe=10$)

Quasi-steady electric field and flow field since time scales are small
in comparison to cycle period and species time scale.

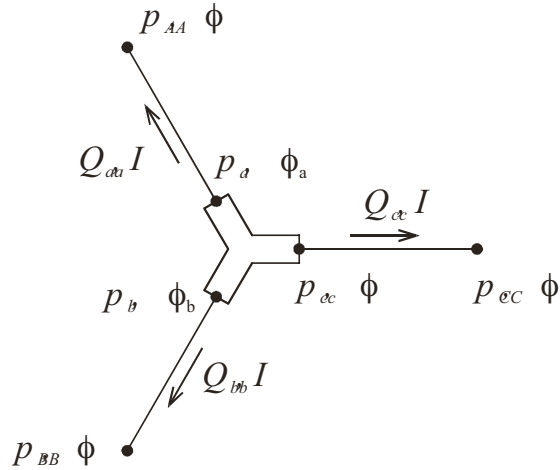
Linking boundary conditions used in the computations.

ICTP Microfluidics 2005, MacInnes

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Case Study 2(2)

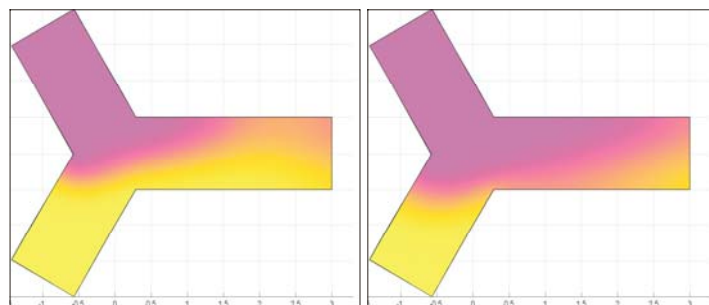
Simple Y-junction

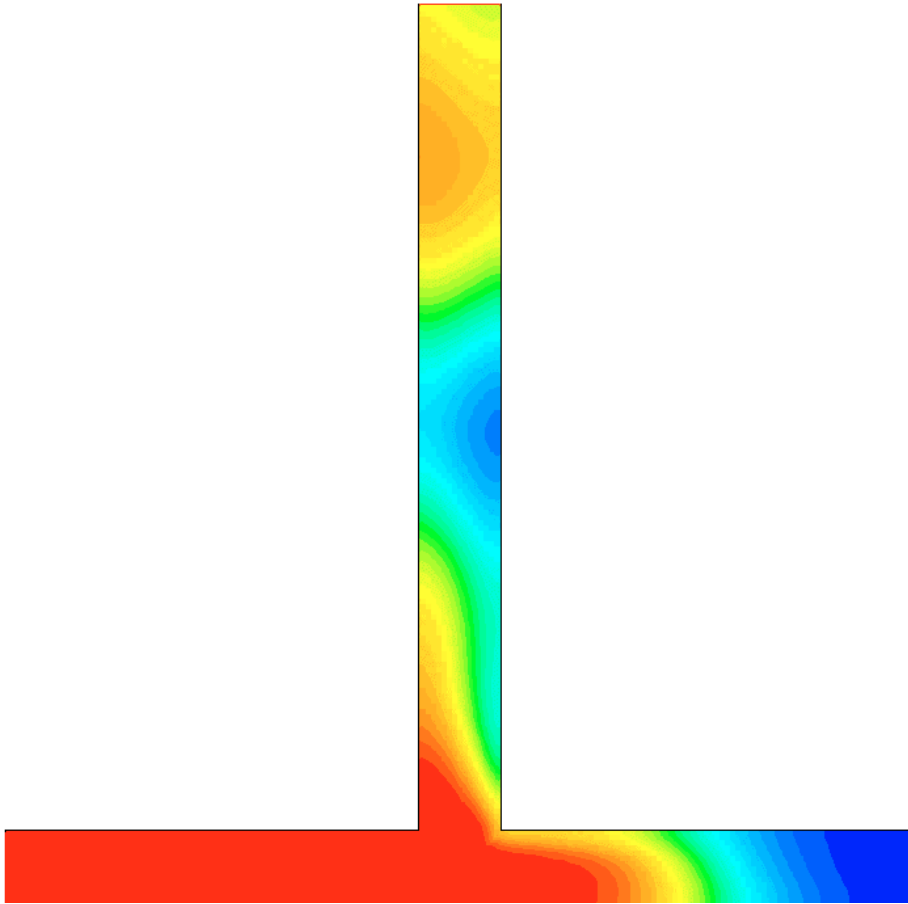


Case Study 2(3)

Simple Y-junction

Composition contours at two times during injection





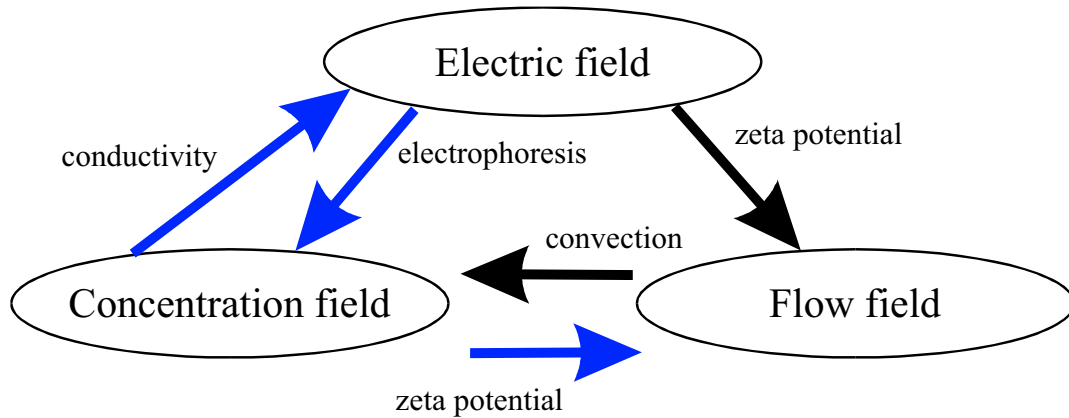
Two issues arise

- 1) Formation of slugs separated by interface normal to the flow
- 2) For chemical reaction, composition will necessarily be non-uniform – this may be expected to result in electrical properties (zeta potential and conductivity)

The first issue is considered later in the lectures with microreactor case studies.

The second issue is considered here since it reveals some further fundamental character and complexity of electrokinetic flows.

Further coupling:

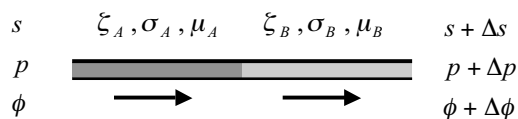


Case Study 3(1)

Effect of non-uniform properties, MacInnes et al., Trans IChemE (2003)

Objective: Verification of species equations, non-uniform properties.
Implications for switching and interfaces.

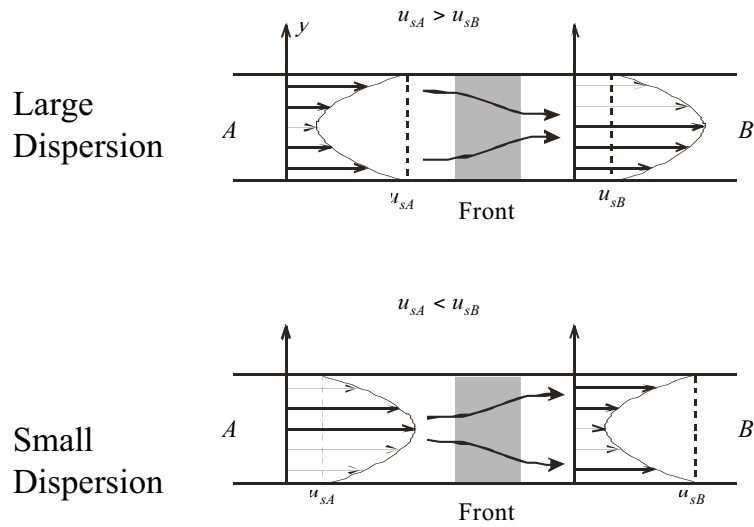
An interface:



Network analysis:

$$\Delta p_A \propto \mu_B \sigma_B \zeta_A - \mu_A \sigma_A \zeta_B$$

Case Study 3(2)

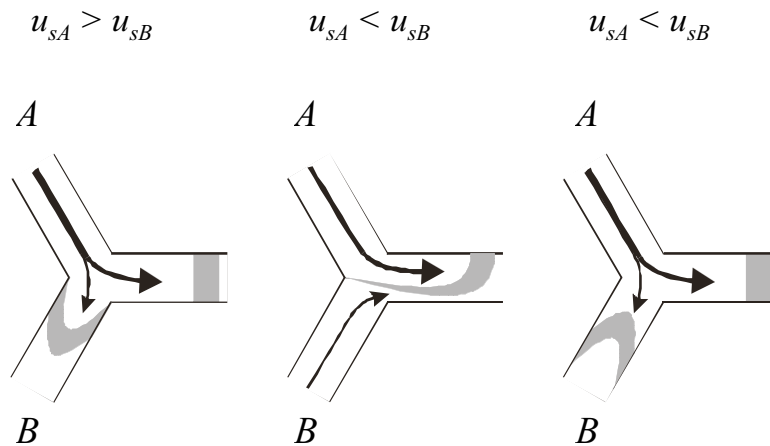


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Case Study 3(3)

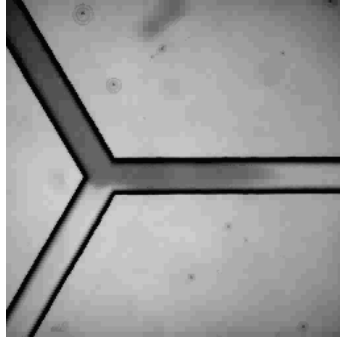
Effect at a junction:



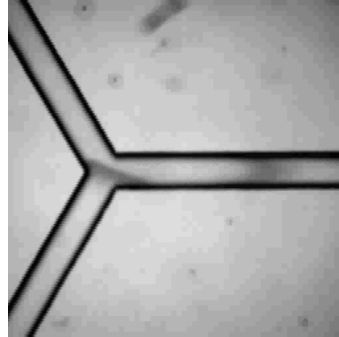
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Y-junction experiment
(PADA + Ni²⁺ → NiPADA²⁺)



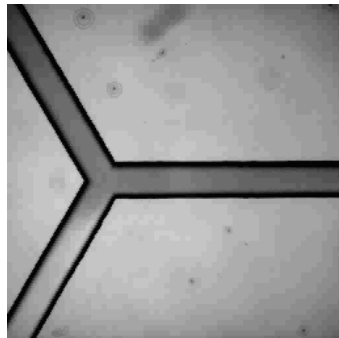
450 nm optical filter



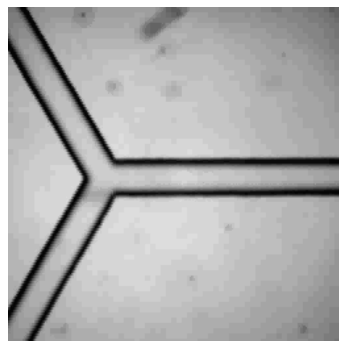
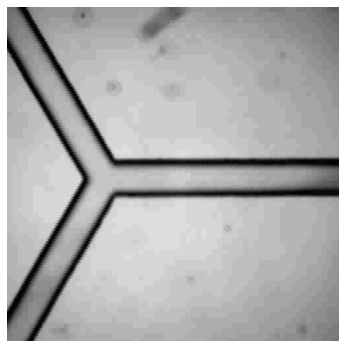
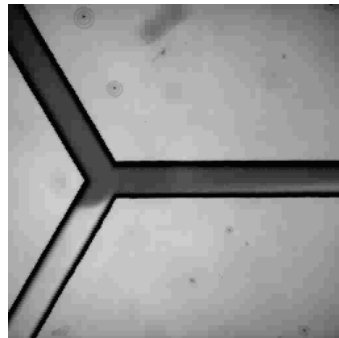
550 nm optical filter

MacInnes, Du and Allen, *IChemE Transactions*, 2003.

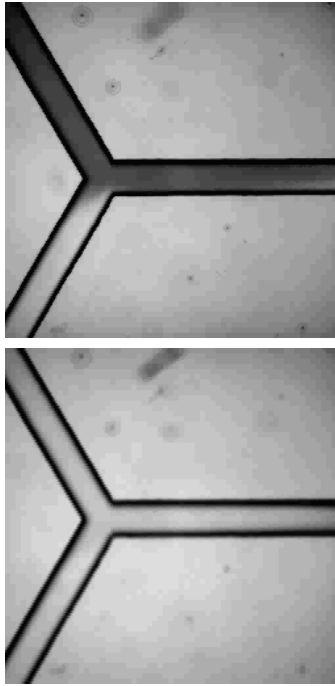
PADA/Ni(NaCl)



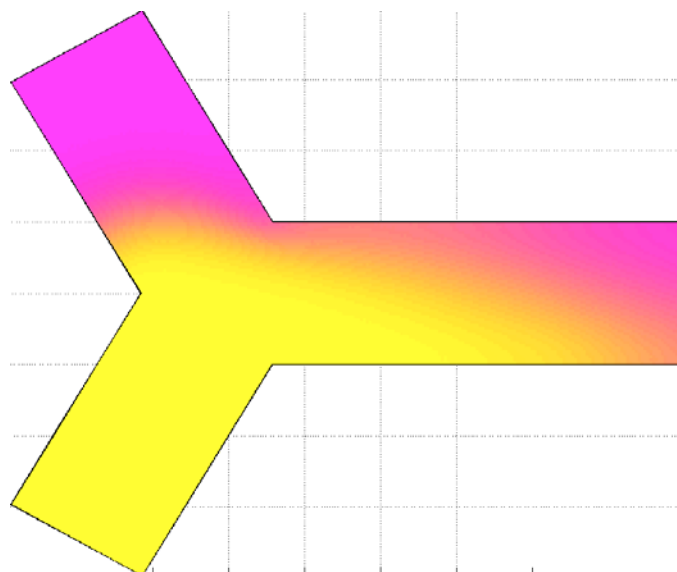
PADA(NaCl)/Ni



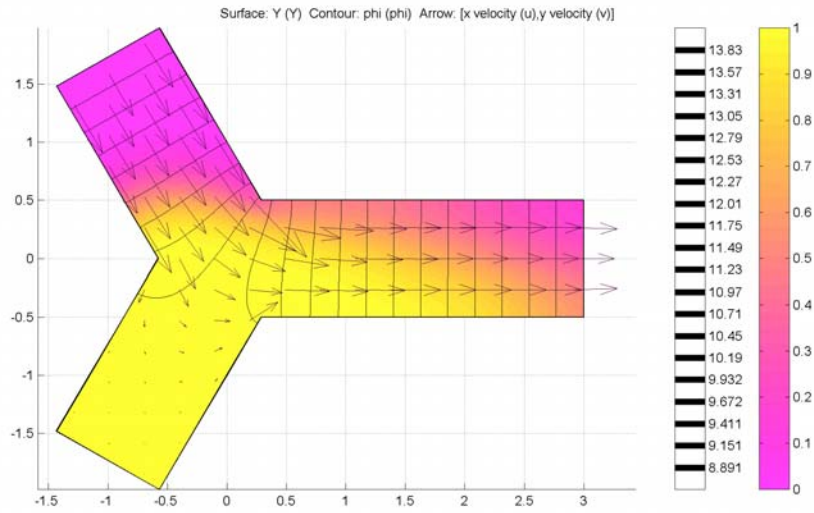
PADA(NaCl)/Ni(NaCl)



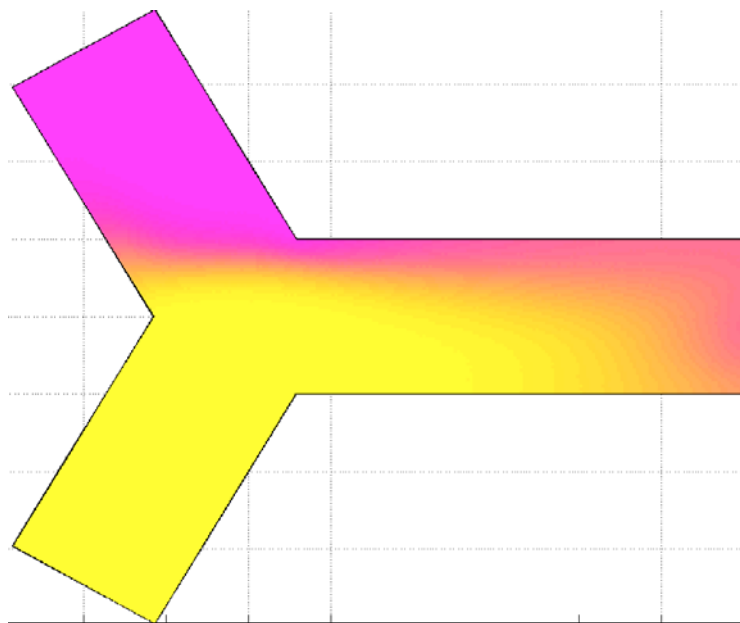
Electric flow, uniform properties



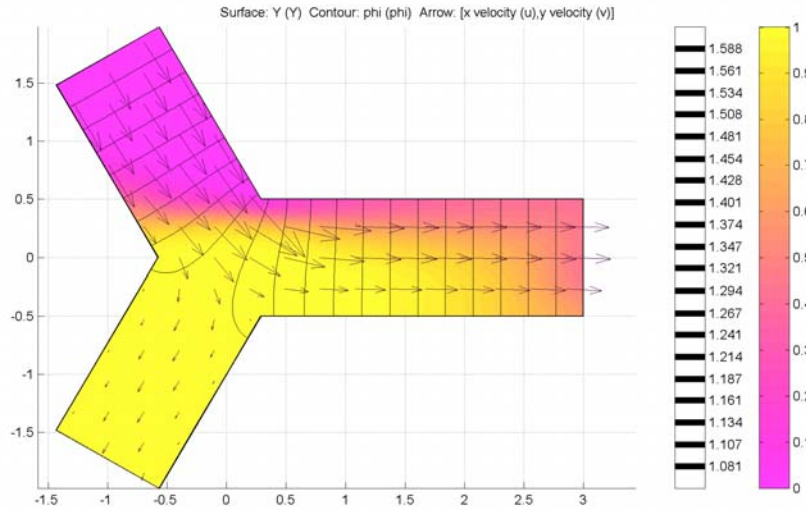
Flow transient



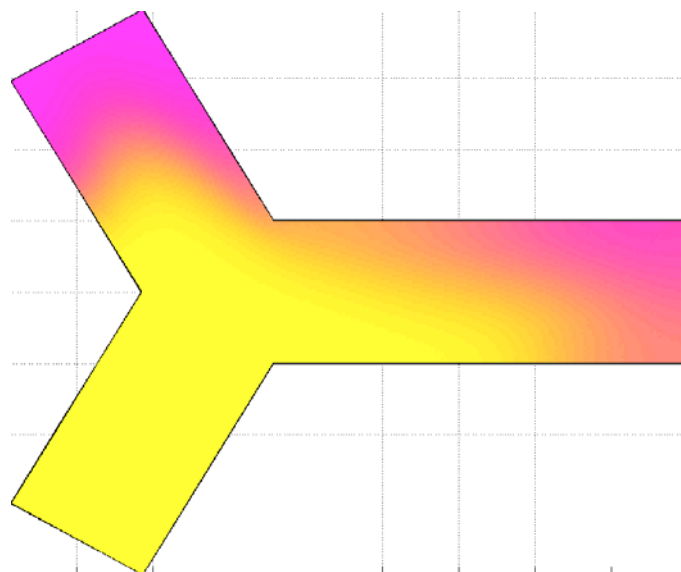
Electric flow, $\zeta_r = 10$



Flow transient



Electric flow, $\sigma_r = 5$



Flow and electric field transient

