Electrohydrodynamic Control in Small Scale Geometries

Meeting on Numerical Challenges in Two-Phase Flows

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Agenda

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Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

Introduction
Motivation

Numerous microfluidic applications require the efficient mixing of fluids, however complications arise in low Reynolds number flows, especially in small scale devices which are difficult to manipulate.

Introduction
Motivation

Electrohydrodynamic
Control in Microfluidics

Radu Cîmpeanu

Introduction
2   Motivation

Mathematical Model
  Geometry
  Governing equations
  Nondimensionalization
  Interfacial and boundary
  conditions

Stability
  Approach

Results
  Numerical package
  Validation
  On-off protocols
  Relay structures
  Polymer Self-Assembly

Conclusions and
Future Directions
  Future goals

Numerous microfluidic applications require the efficient mixing of fluids, however complications arise in low Reynolds number flows, especially in small scale devices which are difficult to manipulate.
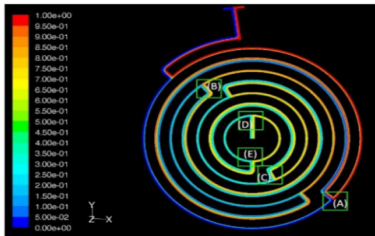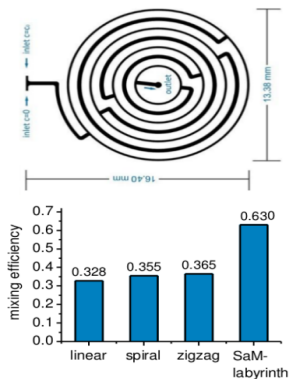
An interesting maze-like configuration has been presented at the 2014 Micro and Nano Flows (MNF) conference by Kefala *et al.*

Introduction
Motivation

Active mixers are the alternative to complex geometrical structures which are often difficult to manufacture and maintain. They employ external forcing (wide varieties thereof exist) in order to encourage mixing, typically in channels.

Introduction
Motivation

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
3   Motivation

Mathematical Model
  Geometry
  Governing equations
  Nondimensionalization
  Interfacial and boundary
  conditions

Stability
  Approach

Results
 Numerical package
  Validation
  On-off protocols
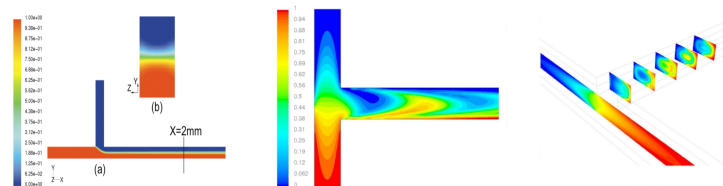 Relay structures
  Polymer Self-Assembly

Conclusions and
Future Directions
  Future goals

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The T-mixer (left, [1]) is one of the most popular experimental devices used, in various geometrical settings and with added effects such as time pulsing (right, [2]).

Introduction
Motivation

Active mixers are the alternative to complex geometrical structures which are often difficult to manufacture and maintain. They employ external forcing (wide varieties thereof exist) in order to encourage mixing, typically in channels.

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In the present work we aim to model efficient electrohydrodynamic control procedures in confined geometries that induce time dependent flows without introducing an imposed velocity field or moving parts.

Mathematical Model

Electrohydrodynamic
Control in Microfluidics

Radu Cîmpeanu

Introduction
Motivation

4 Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
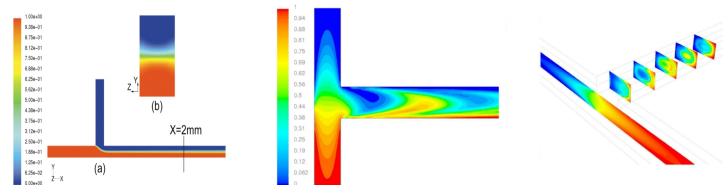Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

Electric fields have been considered in previous studies [3,4] as an efficient means of controlling instabilities arising in some classical flows.

- ▶ The study of interfaces between fluids has received much attention throughout the last decades;
- ▶ High range of applications in classical fluid mechanics, chemical and biological sciences;
- ▶ One of the traditional examples in this field is the Rayleigh-Taylor instability;
- ▶ Imposing a voltage potential difference in a suitable geometrical setting introduces rich dynamics at the microscale, with consequences in many applications.

Mathematical Model - Excursion
Horizontal Electric Fields - RC, DTP and PG Petropoulos, Phys. Fluids, 2014

► Horizontal electric fields (parallel to the fluid-fluid interface) have a stabilising effect on unstably stratified flows.

► The maximum growth rate decreases and the instability shifts to longer and longer wavelengths and can eventually be fully suppressed given a specific wavenumber and tuning the electric field strength.

► Sustained interfacial oscillations?
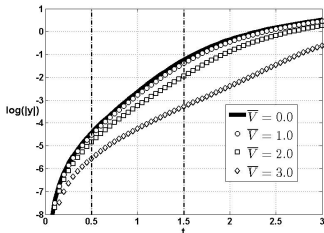
Growth rate extraction.

Validation.

Mathematical Model - Excursion
Horizontal Electric Fields - RC, DTP and PG Petropoulos, Phys. Fluids, 2014

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

6 Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly
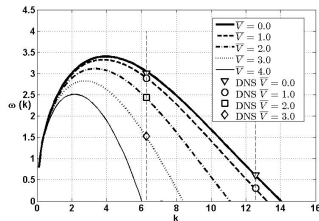
Conclusions and
Future Directions
Future goals

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Mathematical Model
Geometry

Electrohydrodynamic
Control in Microfluidics

Radu Cîmpeanu

Introduction
  Motivation

Mathematical Model
  Geometry
  Governing equations
  Nondimensionalization
  Interfacial and boundary
  conditions

Stability
  Approach

Results
  Numerical package
  Validation
  On-off protocols
  Relay structures
  Polymer Self-Assembly

Conclusions and
Future Directions
  Future goals

Aim: generate efficient mixing of the passive tracer T within the dynamic geometry confined by $y = S(x, t)$ and $y = L/2$ using interfacial dynamics produced by the imposed electric field.

Mathematical Model
Governing equations

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
8 Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
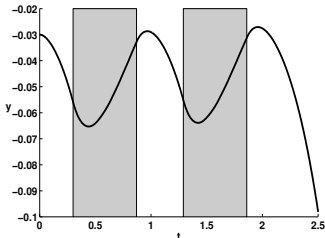Validation
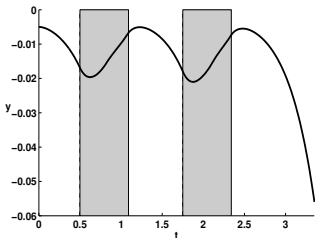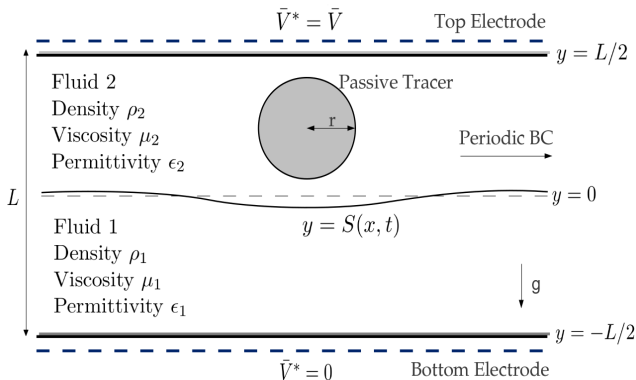On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

The equations for the flow field are the Navier-Stokes equations and the continuity equation for each fluid. In dimensional form the equations are

$$\rho_1(\mathbf{u}_{1t} + (\mathbf{u}_1 \cdot \nabla)\mathbf{u}_1) = -\nabla p_1 + \mu_1 \Delta \mathbf{u}_1 - \rho_1 g \mathbf{j}, \quad (1)$$

$$\rho_2(\mathbf{u}_{2t} + (\mathbf{u}_2 \cdot \nabla)\mathbf{u}_2) = -\nabla p_2 + \mu_2 \Delta \mathbf{u}_2 - \rho_2 g \mathbf{j}, \quad (2)$$

$$\nabla \cdot \mathbf{u}_{1,2} = 0. \quad (3)$$

The electric field equations are given by the Laplace equation for each of the two voltage potentials, one in each fluid

$$\Delta V_{1,2} = 0, \quad (4)$$

with $\Delta \equiv \partial^2/\partial x^2 + \partial^2/\partial y^2$ as the Laplacian operator. The voltage potentials are introduced such that the electric field can then be described by $\mathbf{E}_{1,2} = -\nabla V_{1,2}$.

Mathematical Model
Nondimensionalization

For convenience in notation we introduce the parameters:

$$r = \frac{\rho_1}{\rho_2}, \ m = \frac{\mu_2}{\mu_1}, \ \epsilon = \frac{\epsilon_1}{\epsilon_2}, \quad (5)$$

Assume L to be the width of the channel and U to define the reference velocity. Using $p_1 \sim \rho_1 U^2$ and rescaling by U^2/L, the following dimensionless parameters arise:

$$\tilde{g} = \frac{gL}{U^2}, \ \tilde{\mu} = \frac{\mu_1}{\rho_1 UL}, \ W_e = \frac{\sigma}{\rho_1 gL^2}, \ E_b = \frac{V^2 \epsilon_1}{\rho_1 gL^3} = 1. \quad (6)$$

The absence of a typical velocity in the system encourages the reformulation of the Reynolds number as an inverse Ohnesorge number, such that

$$\mathrm{Re} = \frac{1}{\mathrm{Oh}} = \frac{\sqrt{L\rho_1 \sigma}}{\mu_1}. \quad (7)$$

Mathematical Model
Nondimensionalization

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

With these simplifications, the two Navier-Stokes equations for each of the two fluids now read:

$$\tilde{\mathbf{u}}_{1t} + (\tilde{\mathbf{u}}_1 \cdot \nabla)\tilde{\mathbf{u}}_1 = -\nabla\tilde{p}_1 + \tilde{\mu}\Delta\tilde{\mathbf{u}}_1 - \tilde{g}\mathbf{j}, \qquad (8)$$

$$\tilde{\mathbf{u}}_{2t} + (\tilde{\mathbf{u}}_2 \cdot \nabla)\tilde{\mathbf{u}}_2 = -r\nabla\tilde{p}_2 + m\tilde{\mu}r\Delta\tilde{\mathbf{u}}_2 - \tilde{g}\mathbf{j}. \qquad (9)$$

Here $\mathbf{j}$ denotes the unit vector in vertical direction and (˜) is used throughout the presentation to refer to dimensionless quantities. These equations are naturally complemented by the continuity equation in each fluid:

$$\nabla \cdot \tilde{\mathbf{u}}_{1,2} = 0. \qquad (10)$$

The electric field equations remain unchanged.

Mathematical Model
Interfacial and boundary conditions

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
11 Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

Dept. of Mathematics
Imperial College London
United Kingdom
29

We consider the conditions required at the free surface $y = S(x, t)$

$$\tilde{v}_1 = S_t + \tilde{u}_1 S_x, \ \tilde{v}_2 = S_t + \tilde{u}_2 S_x, \tag{11}$$

$$[\mathbf{n} \cdot \mathcal{T} \cdot \mathbf{n}]_2^1 = \tilde{\sigma} \nabla \cdot \mathbf{n}, \ [\mathbf{t} \cdot \mathcal{T} \cdot \mathbf{n}]_2^1 = 0, \ [\tilde{\mathbf{u}}]_2^1 = 0, \tag{12}$$

From the electrodynamic perspective we only require continuity of voltages across the interface and continuity of the normal component of the displacement field:

$$[V]_2^1 = 0, \ \left[\tilde{\epsilon} \tilde{\mathbf{E}} \cdot \mathbf{n}\right]_2^1 = 0, \tag{13}$$

where $[\cdot]_2^1$ represents the jump in the quantity as the interface is crossed from the lower fluid to the upper fluid. The presence of the walls dictates the necessity of no-slip and impermeability boundary conditions on the velocities, as well as Dirichlet boundary conditions on the electrodes such that

$$\tilde{\mathbf{u}}_1 = 0 \ \text{and} \ V_1 = 0 \ \text{at} \ y = -L/2, \tag{14}$$

$$\tilde{\mathbf{u}}_2 = 0 \ \text{and} \ V_2 = \bar{V} \ \text{at} \ y = +L/2. \tag{15}$$

Stability
Approach

Linearization about the base state solutions is performed via

$$\tilde{V}_1 = \frac{\bar{V}}{\epsilon + 1}(2y + 1) + \delta\hat{V}_1, \quad \tilde{V}_2 = \frac{\bar{V}}{\epsilon + 1}(2\epsilon y + 1) + \delta\hat{V}_2, \tag{16}$$

$$\tilde{p}_1 = -\tilde{g}y + \delta\hat{p}_1, \quad \tilde{p}_2 = -\tilde{g}y/r + \frac{2\bar{V}^2}{(\epsilon + 1)^2}(\epsilon_1 - \epsilon_2\epsilon^2) + \delta\hat{p}_2 \tag{17}$$

$$\tilde{\mathbf{u}}_{1,2} = \delta\hat{\mathbf{u}}_{1,2}, \quad S = \delta\hat{S}, \tag{18}$$

with δ considered to be sufficiently small. We assume normal mode solutions

$$\hat{V}_{1,2}(x, y, t) = \breve{V}_{1,2}(y)e^{ikx + \omega t}, \tag{19}$$

$$\hat{p}_{1,2}(x, y, t) = \breve{p}_{1,2}(y)e^{ikx + \omega t}, \tag{20}$$

$$\hat{\mathbf{u}}_{1,2}(x, y, t) = \breve{\mathbf{u}}_{1,2}(y)e^{ikx + \omega t}, \tag{21}$$

$$\hat{S}(x, t) = \breve{S}e^{ikx + \omega t}. \tag{22}$$

We then substitute the formulas into our entire system of equations and boundary conditions and retrieve a system of nine homogeneous equations to be solved for nine unknown constants.

Results
Numerical package

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

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United Kingdom

For both validation of theoretical results and nonlinear computations, we use the Gerris Flow Solver, a highly versatile volume-of-fluid package, designed with multiphysics problem solving capabilities.
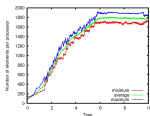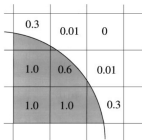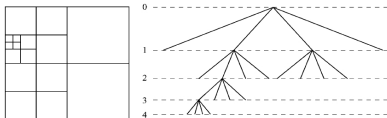

```
# shift the origin of the reference box to (0,0)
2 1 GfsRiver GfsBox GfsGEdge { x = 0.5 y = 0.5 } {
  # the domain is 3.402 m X 6.804 m
  # units for time are seconds
  PhysicalParams { L = 3.402 g = 9.81 }
  Refine 6

  # maintain the Zb1 variable using the GTS surface
  VariableFunction Zb1 bathy.gts

  # the initial water level is at z = 0, so the depth P is...
  Init {} {
    P = MAX (0., -Zb1)
  }

  # use a Sweby limiter rather than the default minmod which is too
  # dissipative
  AdvectionParams { gradient = gfs_center_sweby_gradient }

  # adapt down to 9 levels based on the slope of the (wet)
  # free-surface and with a tolerance of 1 mm
  AdaptGradient { istep = 1 } {
    cmax = 1e-3
    cfactor = 2
    maxlevel = 9
    minlevel = 6
  } (P < DRY ? 0. : P + Zb)

  # at each timestep
  Init { istep = 1 } {
    # Add a "shelf" to simulate the wall on the right-hand side boundary
    Zb = (x > 5.448 ? 0.13535 : Zb)
    # read in the experimental timeseries in variable 'input'
    input = input.cgd
    # implicit quadratic bottom friction with coefficient 1e-3
    U = (P > DRY ? U/(1. + dt*1e-3*Velocity/P) : 0.)
    V = (P > DRY ? V/(1. + dt*1e-3*Velocity/P) : 0.)
    P = (P > DRY ? P : 0.)
  }
```

Results
Realistic fluid setup

Property [units]	Water at $25°$C	Olive oil at $25°$C
Density [$\mathrm{kg/m^3}$]	998	918
Viscosity [$\mathrm{Pa \cdot s}$]	$8.95 \cdot 10^{-4}$	0.081
Permittivity [$\mathrm{kg^{-1}s^4A}$]	$80.4\epsilon_0$	$3.1\epsilon_0$

- ϵ_0 is the permittivity of free space, $8.85 \cdot 10^{-12}$ $\mathrm{m^{-3}kg^{-1}s^4A^2}$.

- The surface tension between olive oil and water is 0.02 $\mathrm{kg \cdot s^{-2}}$.

- We use a channel of height 0.01 m under the action of a gravitational acceleration of 9.80655 $\mathrm{m \cdot s^{-2}}$.

- A strong destabilization of the system occurs for an electric field strength $E_c \approx 10^5$ V/m for a large array of wavenumbers of the initial perturbation.

- Electric breakdown value for water: $E \approx 1.35 \cdot 10^7$ V/m; $E \approx 1.755 \cdot 10^7$ V/m for olive oil.

Results
Validation

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
15 **Validation**
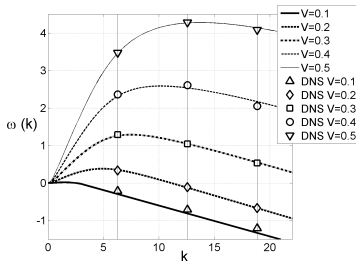On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

▶ Numerical validation of the linear theory has been performed via direct numerical simulation for several test cases.

▶ The growth rates have been extracted using sliding least squares methods.

▶ Excellent agreement is found between linear theory and the early stages of the full computational experiments.

▶ For this verification, we have chosen parameters:
$r = \rho_1/\rho_2 = 1.087$,
$m = \mu_2/\mu_1 = 90.5$,
$\epsilon = \epsilon_1/\epsilon_2 = 25.93$,
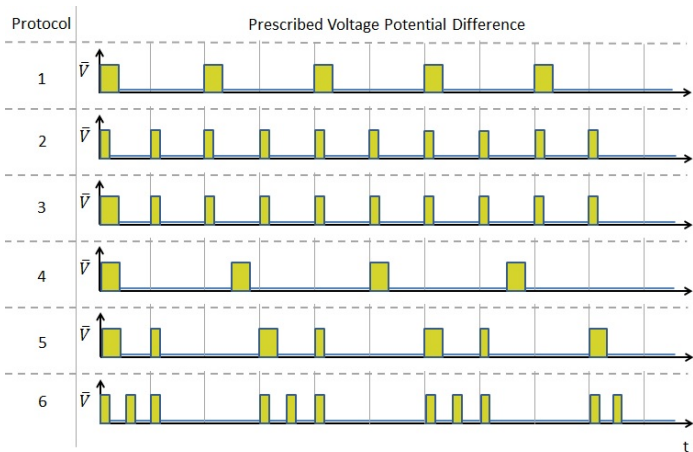$\tilde{\mu} = 4.4 \cdot 10^{-4}$, $\tilde{\sigma} = 0.0362$
and $\bar{V} = 0.1$ to 0.5.

▶ This corresponds to an $\mathcal{O}(1)$ mm-sized system (7.5 mm) subjected to electric fields of up to 10^7 V/m.

Results
On-off protocols - RC and DTP, Proc. MNF, 2014

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

A strong destabiziling uniform electric field is imposed in order to generate interfacial dynamics that enhances mixing within the confined geometry.

Results
On-off protocols - RC and DTP, Proc. MNF, 2014

Given variance of the concentration field in the domain σ, define

$$\text{degree of mixing} = 1 - \frac{\sigma^2(t)}{\sigma^2_{max}}, \qquad (23)$$

where σ^2_{max} is the variance of the perfectly segregated state [7]. The variance is naturally defined as $\sigma^2(t) = <c^2(t)> - <c(t)>^2$, where c denotes the entire concentration field at time t.

Results
On-off protocols

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly
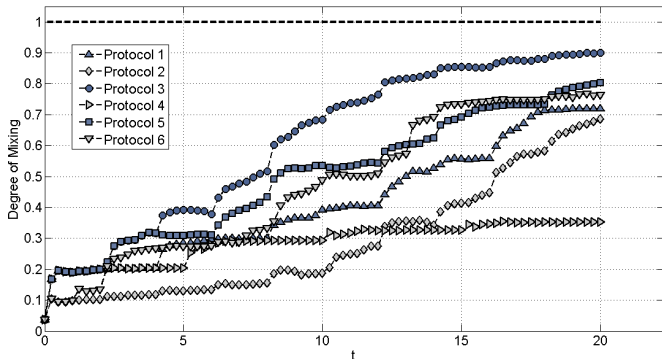
Conclusions and
Future Directions
Future goals

Using the same type of metrics for the degree of mixing, we return to the case of the realistic fluid setup (water-oil system) and propose a generalisation of the previous protocol to

$$
V_2(x, L/2, t) =
\begin{cases}
C + Ax + \dfrac{A}{2}\left(-\dfrac{2}{\pi}\tan^{-1}(\delta'(x + 0.5)) - \right. \\
\qquad\qquad \left. -\dfrac{2}{\pi}\tan^{-1}(\delta'(x - 0.5)) \right) \text{ if } t_{on}, \\
0 \text{ if } t_{off},
\end{cases}
$$

▶ This acts as a dielectrophoretic adjustment, in which C is the background voltage potential difference and constant parameter A dictates the slope of the linear variation of the electric field across the geometry.

▶ The imposition of periodic boundary conditions in the horizontal directions require a special handling of the endpoints, which prompts the usage of a special smoothing function, generating a voltage distribution without discontinuities.

Results
On-off protocols

Electrohydrodynamic
Control in Microfluidics

Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
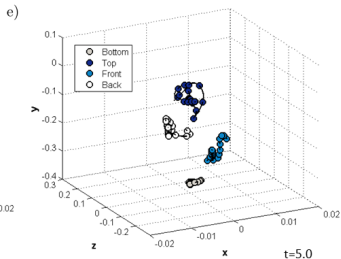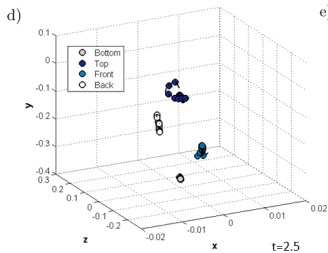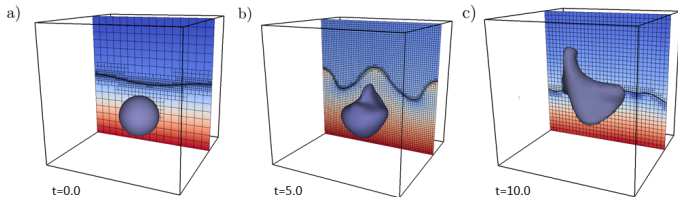Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

By varying t_{on}-t_{off} intervals, as well as parameter A, we create a series of eight electric field protocols that act on the realistic fluid setup.
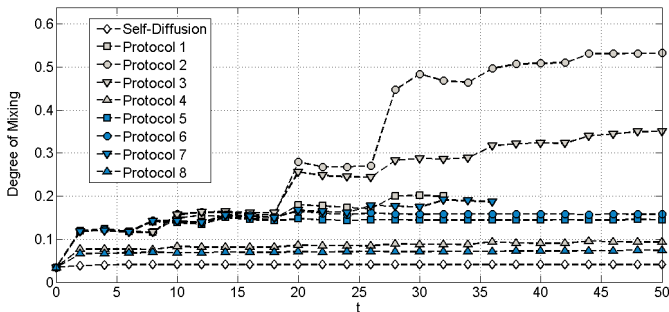
The degree of mixing is however not the only method of assessing the performance of the proposed electric field protocols.

Microfluidic Mixing
On-off protocols in three dimensions - symmetric case

Microfluidic Mixing
On-off protocols in three dimensions - asymmetric case

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

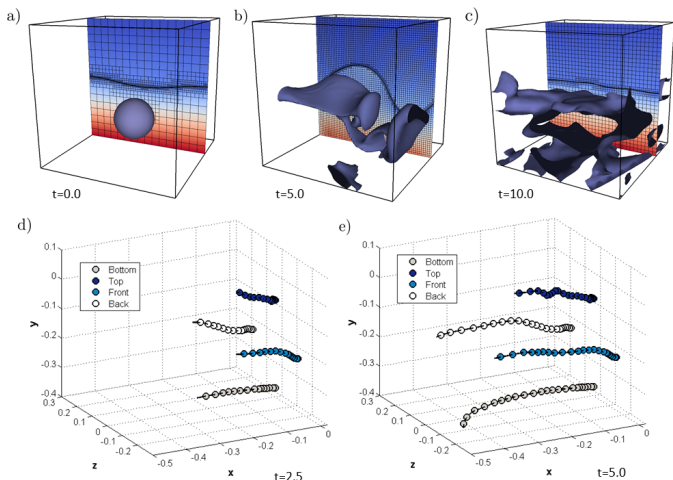Results
Numerical package
Validation
21 On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

Relay structures
Construction - RC and DTP, Royal Soc. Phil. Trans. A, 2014

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
22 Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

We also propose a mechanism for introducing pumping by generating a travelling wave voltage distribution on one or both of the electrodes [5,6], with different imposed properties (velocity, amplitude).
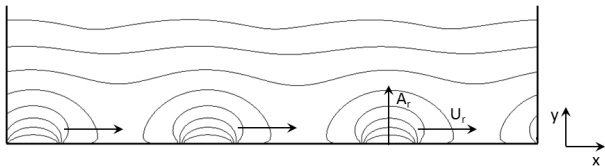
A Dirichlet boundary condition of the following type can be used

$$\bar{V}(t) = C + \frac{2A_r}{\pi}\left[\tan^{-1}\left(\frac{x - x_L - U_r t}{\delta'}\right) - \tan^{-1}\left(\frac{x - x_R - U_r t}{\delta'}\right)\right],$$

making sure the electrostatic approximation is still valid. We monitor the induced flux in the flow via

$$F(t) = \int_{-0.5}^{+0.5} u(0, y, t)dy. \qquad (24)$$

Relay structures
Flux generation I - RC and DTP, Royal Soc. Phil. Trans. A, 2014

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
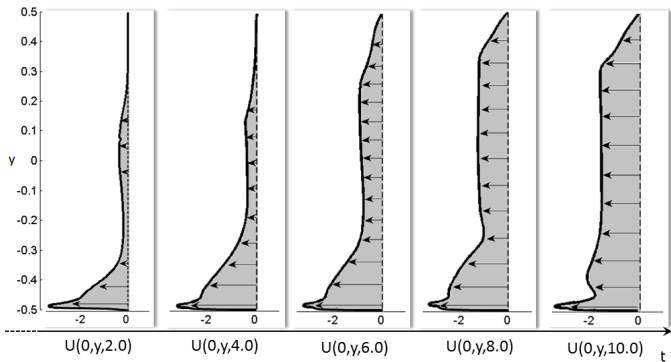Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

The velocity profiles become more pronounced as we advance in time. The effects from the lower part of the domain (where the boundary condition is imposed) are gradually transmitted to the entire channel.

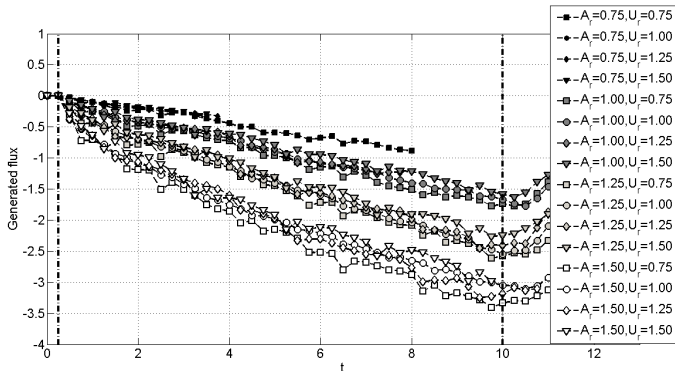# Relay structures
Flux generation II - RC and DTP, Royal Soc. Phil. Trans. A, 2014

Electrohydrodynamic
Control in Microfluidics

Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
24 Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

A careful analysis of several test cases reveals that the amplitude of the travelling wave is the primary factor contributing to the pumping effect, while the velocity itself plays a secondary role within the parameter range considered.

Polymer Self-Assembly
Motivation

Electrohydrodynamic
Control in Microfluidics

Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

25

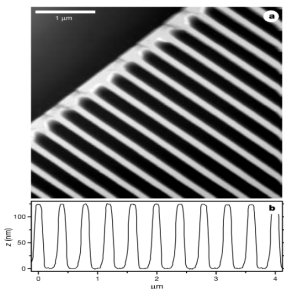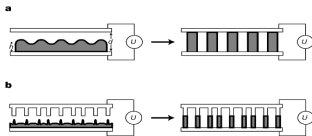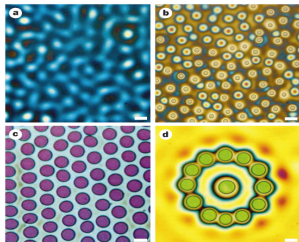Conclusions and
Future Directions
Future goals

Electric field effects in small geometries have also been studied in the context of polymer self-assembly and integrated circuit component construction, proving remarkable versatility.

Electrically induced structure formation and pattern transfer

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† Polymer Science and Engineering Department, University of Massachusetts at Amherst, Amherst, Massachusetts 01003, USA
‡ Department of Polymer Chemistry, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Conclusions and Future Directions
Closing remarks

The existing project was focused on the following objectives:

▶ the construction of a mathematical framework for the study of the Rayleigh-Taylor instability in an electrohydrodynamical context in small scale geometries;

▶ the usage of high-performance specialised numerical software capable of capturing the physical behavior of the studied model;

▶ the rigorous testing of both linear and nonlinear scenarios, highlighting some key features in the flow;

▶ the modeling of efficient electrically induced mixing protocols that could be used in experimental setups.

Conclusions and Future Directions
Future goals

The most relevant extensions to the present research are directed towards the generalization of the current machinery. Possible applications include:

- ▶ extension of the physical domain to different types of channels;
- ▶ improved performance and manipulation of the relay structures;
- ▶ integration of previosuly described protocols in devices such as time pulsed T-mixers;
- ▶ concrete physical applications with real world fluid models and (possibly) experimental studies;
- ▶ improvement of the numerical package Gerris in order to be able to capture the relevant information in the previous suggestions.

Conclusions and Future Directions
Selected references

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
Future goals

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Conclusions and Future Directions
Acknowledgements and contact information

Electrohydrodynamic
Control in Microfluidics
Radu Cîmpeanu

Introduction
Motivation

Mathematical Model
Geometry
Governing equations
Nondimensionalization
Interfacial and boundary
conditions

Stability
Approach

Results
Numerical package
Validation
On-off protocols
Relay structures
Polymer Self-Assembly

Conclusions and
Future Directions
29   Future goals

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Thank you for your attention

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