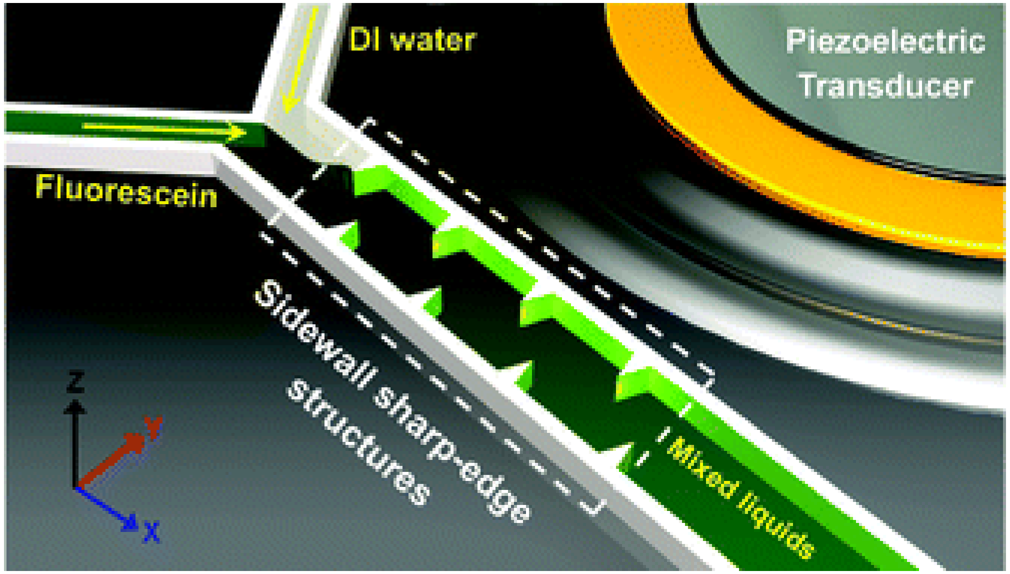
COMSOL CONFERENCE 2015 BOSTON

Acoustic Streaming Driven Mixing



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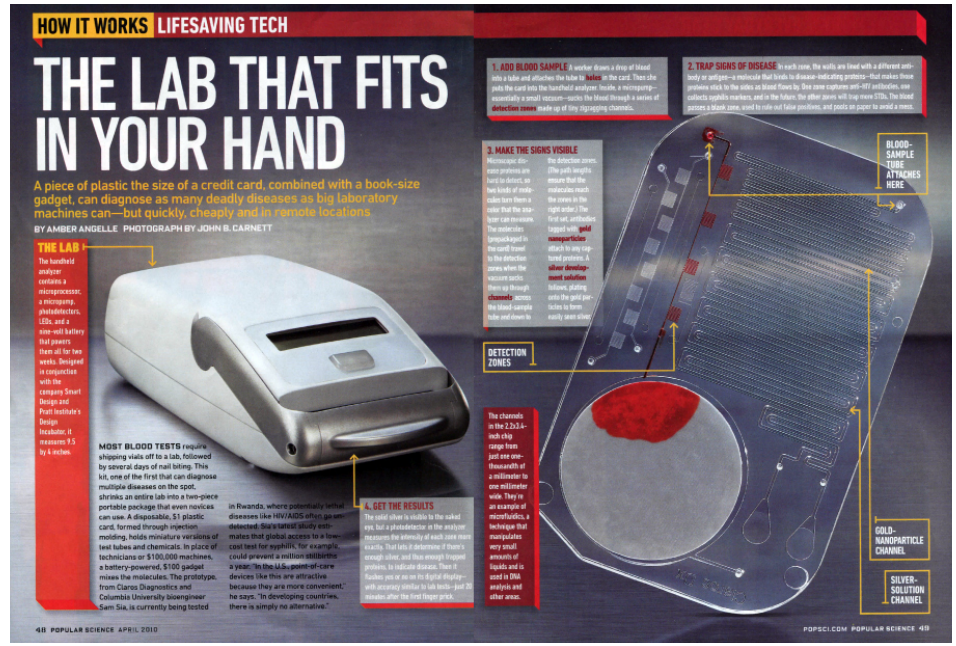
Outline

- Motivation
- Introduction to sharp-edge based micromixer
- Numerical scheme
- COMSOL Modeling and convergence
- Results
- Conclusion and Outlook

Motivation – Lab on a chip

Lab on a chip (LOC) – A device that integrates one or several of the laboratory functions onto a small chip.


HOW IT WORKS LIFESAVING TECH

THE LAB THAT FITS IN YOUR HAND

A piece of plastic the size of a credit card, combined with a book-size gadget, can diagnose as many deadly diseases as big laboratory machines can—but quickly, cheaply and in remote locations

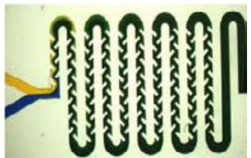
BY AMBER ANGELLE PHOTOGRAPH BY JOHN B. CARNETT

- Low-cost.
- Faster results.
- Low sample consumption.
- Point-of-care diagnostics.
- Ease of operation.

Microfluidics towards lab-on-a-chip

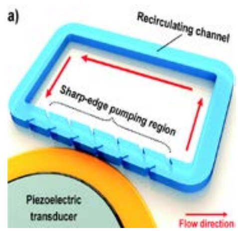
Common functionalities needed:

- **Fluid manipulation**
  - Mixing



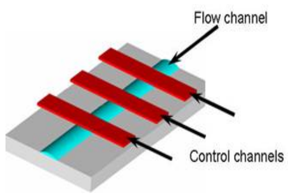
Kwona et al, *Tetrahedron Letters,* 2008

  - Pumping



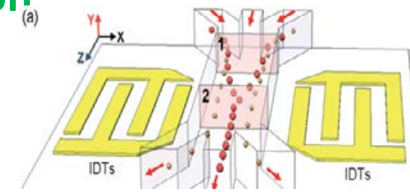
Huang et al, Lab on a Chip, 2014.

  - Valves



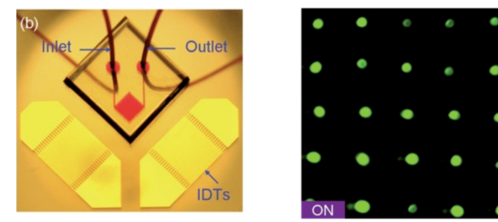
Melin et al, Ann. Rev. Biophys., 2007.

- **Particle/Cell manipulation**
  - Separation



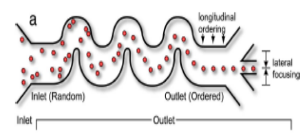
Shi et al, Lab on a Chip, 2009.

  - Patterning

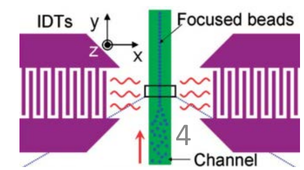


Shi et al, Lab on a Chip, 2009.

  - Focusing



Di Carlo, PNAS, 2007.



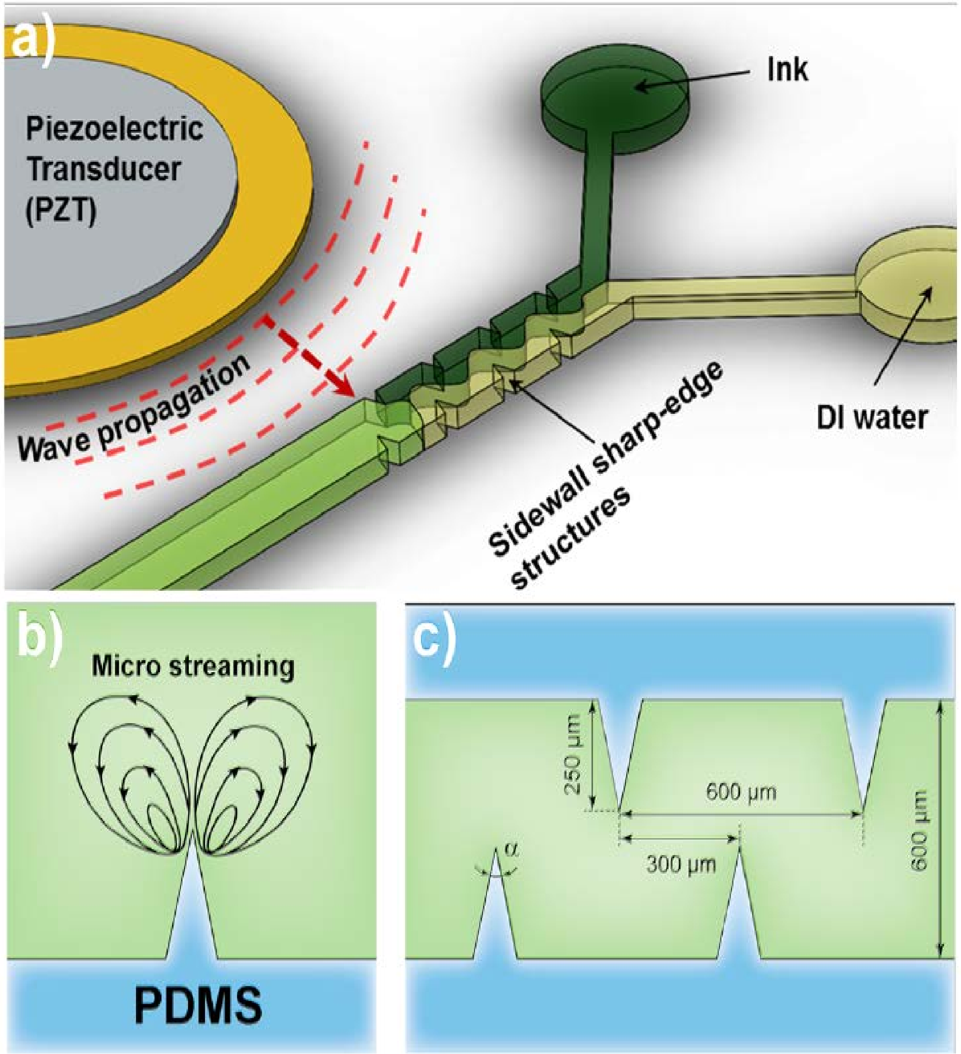
Shi et al, Lab on a Chip, 2007.

Challenges at microscales:

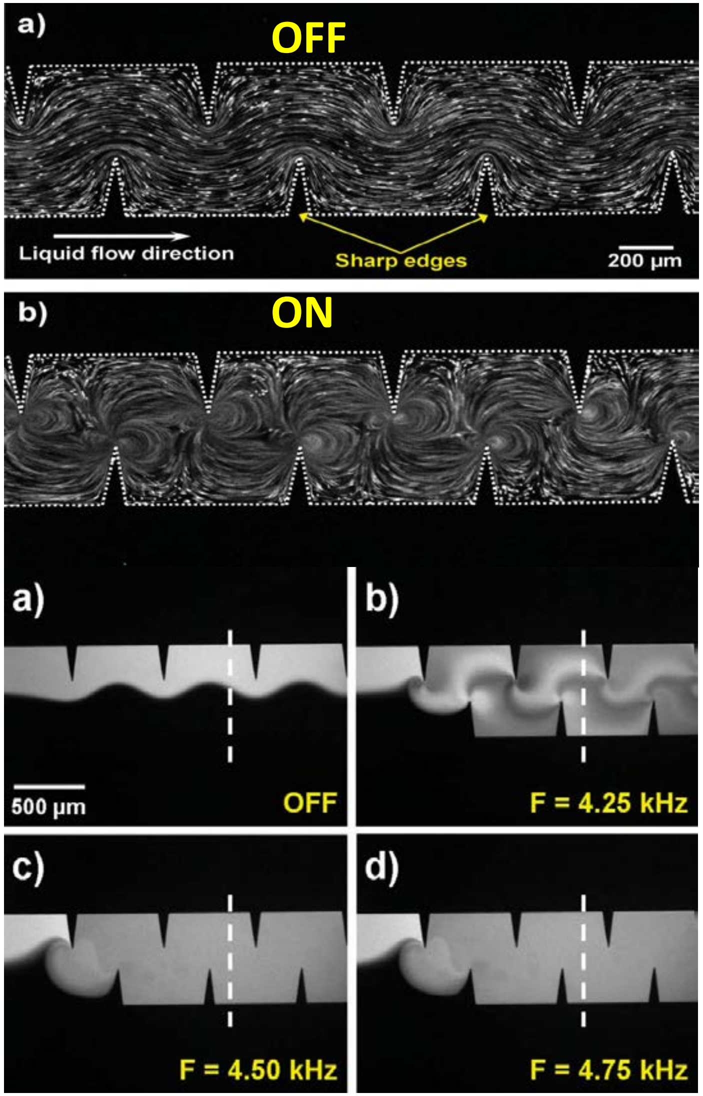
- Low Reynolds number ⇒ Slow diffusion dominated mixing
- Difficult fluid pumping

$$\Delta P = \frac{8\mu L Q}{\pi r^4}$$

Sharp-edge based microfluidic mixing



Nama et al, Lab on a Chip, 2014.



Huang et al, Lab on a Chip, 2014.

Governing equations

Balance of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

Balance of linear momentum

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla p + \mu \nabla^2 \mathbf{v} + \left(\mu_b + \frac{1}{3} \mu \right) \nabla (\nabla \cdot \mathbf{v})$$

Constitutive relation

$$p = {c_0}^2 \rho$$

Convection-Diffusion Equation

$$\frac{\partial c}{\partial t} + \boldsymbol{\nabla} \cdot (c\boldsymbol{v}) = D \nabla^2 c$$

Numerical Challenges associated with direct solution:

- Widely separated length scales – Characteristic wavelengths (1 m) vs. characteristic dimensions of microfluidic channel (10^{-3} m)
- Widely separated time scales – Characteristic oscillation period (10^{-4} s) vs. characteristic times dictated by streaming speeds (10^{-1} s)
- Direct simulations are possible, but are computationally expensive.

Numerical Model

Perturbation expansion

$$\mathbf{v} = \mathbf{v}_0 + \varepsilon \tilde{\mathbf{v}}_1 + \varepsilon^2 \tilde{\mathbf{v}}_2 + O(\varepsilon^3) + \cdots$$

$$p = p_0 + \varepsilon \tilde{p}_1 + \varepsilon^2 \tilde{p}_2 + O(\varepsilon^3) + \cdots$$

$$\rho = \rho_0 + \varepsilon \tilde{\rho}_1 + \varepsilon^2 \tilde{\rho}_2 + O(\varepsilon^3) + \cdots$$

- Presence of a background laminar flow before actuation

Zeroth-order equations

$$\frac{\partial \rho_0}{\partial t} + \rho_0(\boldsymbol{\nabla} \cdot \boldsymbol{v}_0) = 0,$$

$$\rho_0 \frac{\partial \boldsymbol{v}_0}{\partial t} + \rho_0(\boldsymbol{v}_0 \cdot \boldsymbol{\nabla})\boldsymbol{v}_0 = -\boldsymbol{\nabla} p_0 + \mu \nabla^2 \boldsymbol{v}_0 + (\mu_b + \tfrac{1}{3}\mu)\boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{v}_0).$$

First-order equations

$$\frac{\partial \rho_1}{\partial t} + \boldsymbol{\nabla} \cdot (\rho_0 \boldsymbol{v}_1 + \rho_1 \boldsymbol{v}_0) = 0,$$

$$\rho_0 \frac{\partial \boldsymbol{v}_1}{\partial t} + \rho_1 \frac{\partial \boldsymbol{v}_0}{\partial t} + \rho_0(\boldsymbol{v}_1 \cdot \boldsymbol{\nabla})\boldsymbol{v}_0 + \rho_0(\boldsymbol{v}_0 \cdot \boldsymbol{\nabla})\boldsymbol{v}_1 + \rho_1(\boldsymbol{v}_0 \cdot \boldsymbol{\nabla})\boldsymbol{v}_0 = -\boldsymbol{\nabla} p_1 + \mu \nabla^2 \boldsymbol{v}_1 + (\mu_b + \tfrac{1}{3}\mu)\boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{v}_1).$$

Numerical Model

Second-order equations

$$\left\langle \frac{\partial \rho_2}{\partial t} \right\rangle + \boldsymbol{\nabla}\cdot(\langle \rho_0 \boldsymbol{v}_2 \rangle + \langle \rho_2 \boldsymbol{v}_0 \rangle) = -\boldsymbol{\nabla}\cdot\langle \rho_1 \boldsymbol{v}_1 \rangle,$$

$$\left\langle \rho_0 \frac{\partial \boldsymbol{v}_2}{\partial t} \right\rangle + \left\langle \rho_2 \frac{\partial \boldsymbol{v}_0}{\partial t} \right\rangle + \left\langle \rho_1 \frac{\partial \boldsymbol{v}_1}{\partial t} \right\rangle + \langle \rho_0 \boldsymbol{v}_1 \cdot \boldsymbol{\nabla} \boldsymbol{v}_1 \rangle$$
$$+ \langle \rho_0 \boldsymbol{v}_0 \cdot \boldsymbol{\nabla} \boldsymbol{v}_2 \rangle + \langle \rho_0 \boldsymbol{v}_2 \cdot \boldsymbol{\nabla} \boldsymbol{v}_0 \rangle + \langle \rho_1 \boldsymbol{v}_0 \cdot \boldsymbol{\nabla} \boldsymbol{v}_1 \rangle$$
$$+ \langle \rho_1 \boldsymbol{v}_1 \cdot \boldsymbol{\nabla} \boldsymbol{v}_0 \rangle + \langle \rho_2 \boldsymbol{v}_0 \cdot \boldsymbol{\nabla} \boldsymbol{v}_0 \rangle$$
$$= -\boldsymbol{\nabla} \langle p_2 \rangle + \mu \nabla^2 \langle \boldsymbol{v}_2 \rangle + (\mu_b + \tfrac{1}{3}\mu) \boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\langle \boldsymbol{v}_2 \rangle)$$

Convection-Diffusion Equation

$$\frac{\partial c}{\partial t} + \boldsymbol{\nabla}\cdot(c\boldsymbol{v}) = D\nabla^2 c$$

Stoke’s Drift

Mean Lagrangian Velocity

$$\boldsymbol{v}^{\mathrm{L}} = \langle \boldsymbol{v}_2 \rangle + \langle (\boldsymbol{\xi}_1 \cdot \nabla) \boldsymbol{v}_1 \rangle$$

$$\frac{\partial \boldsymbol{\xi}_1}{\partial t} = \boldsymbol{v}_1$$

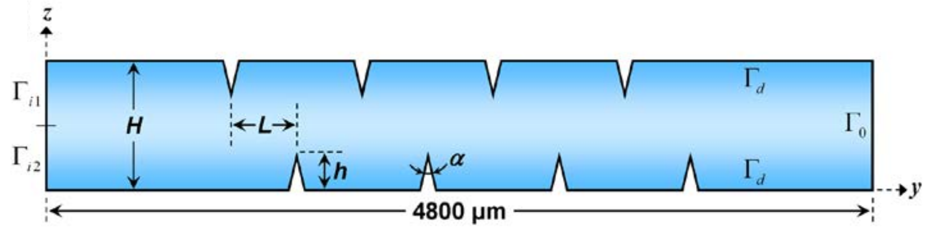
Effective convection velocity

$$\boldsymbol{v}^{\mathrm{C}} = \boldsymbol{v}_0 + \boldsymbol{v}^{\mathrm{L}}$$

Boundary Conditions

Zeroth-order: $\boldsymbol{v}_0 = \boldsymbol{v}_{in}, \quad \text{on} \quad \Gamma_{i1} \cup \Gamma_{i2}.$

$$\boldsymbol{v}_0 = \boldsymbol{0}, \quad \text{on} \quad \Gamma_d$$



First-order:

Harmonic Displacement $u_y(z) = d_0 + d_0\left(\frac{z}{h}\right)^3$

$$\boldsymbol{v}_1(t,z) = \frac{\partial \boldsymbol{u}(t,z)}{\partial t}, \quad \text{on} \quad \Gamma_d$$

Second-order: $\boldsymbol{v}_2 = \boldsymbol{0}, \quad \text{on} \quad \Gamma_d$

Convection-Diffusion Equation: $c = 0, \quad \text{on} \quad \Gamma_{i1}.$

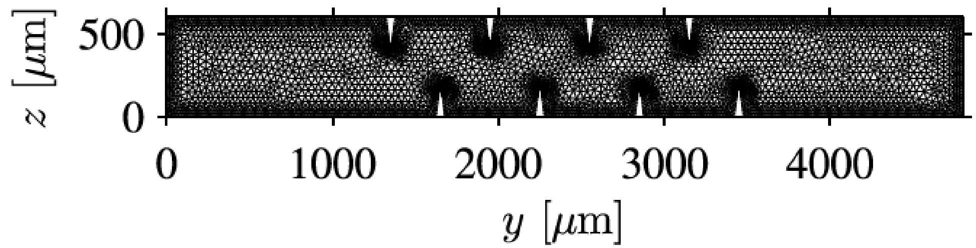
$$c = 1\ mol/m^3, \quad \text{on} \quad \Gamma_{i2}$$

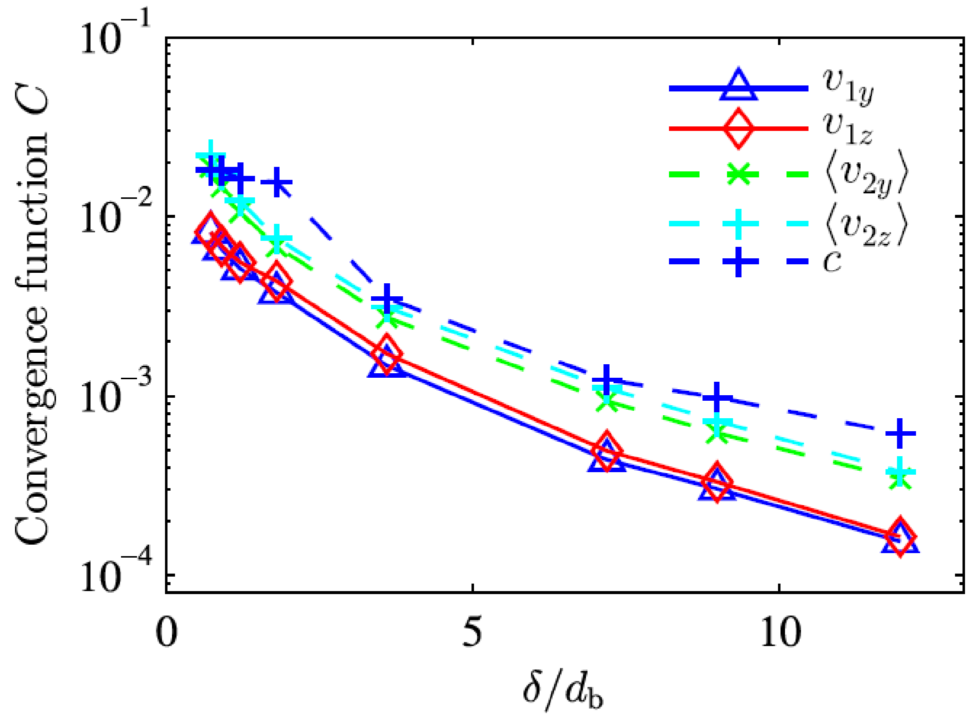
No flux at walls $c\boldsymbol{v} = \boldsymbol{0}, \quad \text{on} \quad \Gamma_d$

Outlet $c\boldsymbol{v} - D\nabla c = \boldsymbol{0}, \quad \text{on} \quad \Gamma_o$

COMSOL Modeling and convergence

- *Weak PDE* interface
- P2/P1 elements for velocity and pressure.
- The sharp corners were rounded off with a small radius using *Fillet*
- *Parametric sweep* for the mesh size to obtain mesh convergence.
- Finer mesh near the boundaries to resolve the boundary layers.

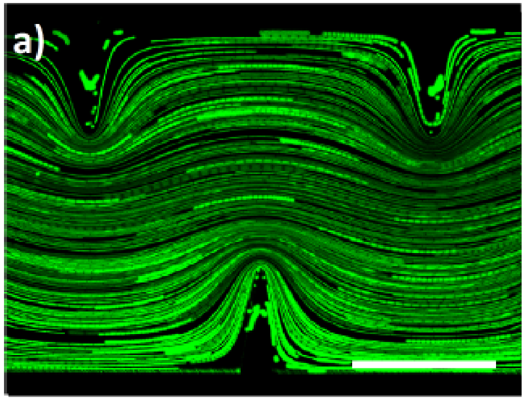


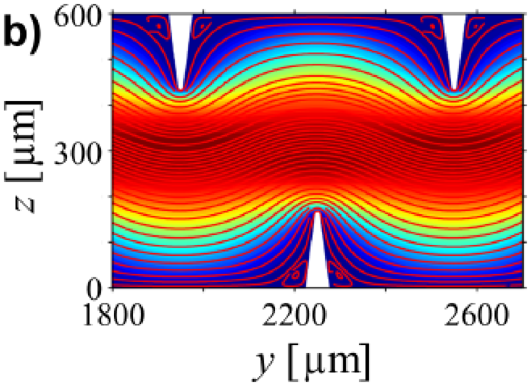


$$C(g) = \sqrt{\frac{\int (g - g_{\text{ref}})^2 \, \mathrm{d}y \, \mathrm{d}z}{\int (g_{\text{ref}})^2 \, \mathrm{d}y \, \mathrm{d}z}}$$

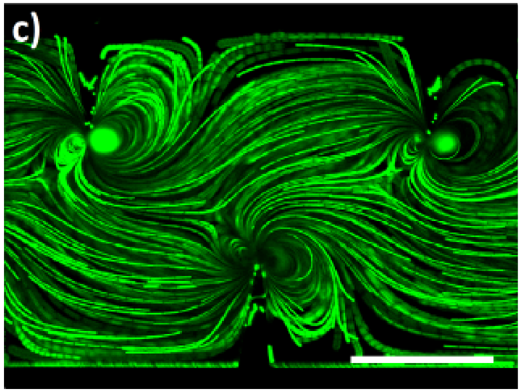
Comparison with Experiments

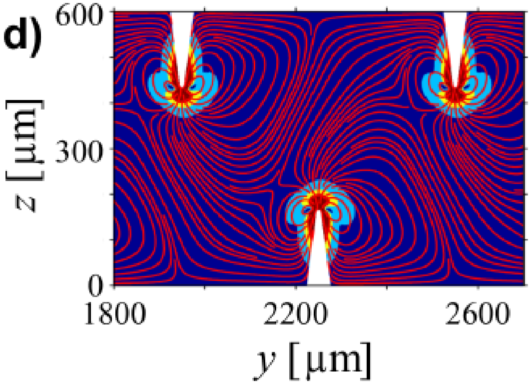
ACOUSTICS OFF



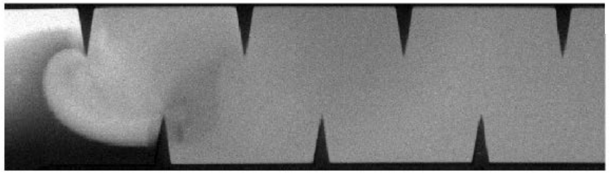


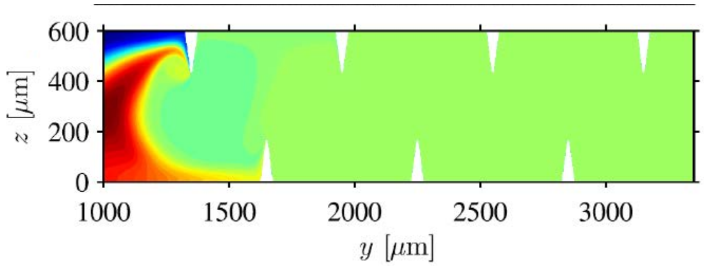
ACOUSTICS ON



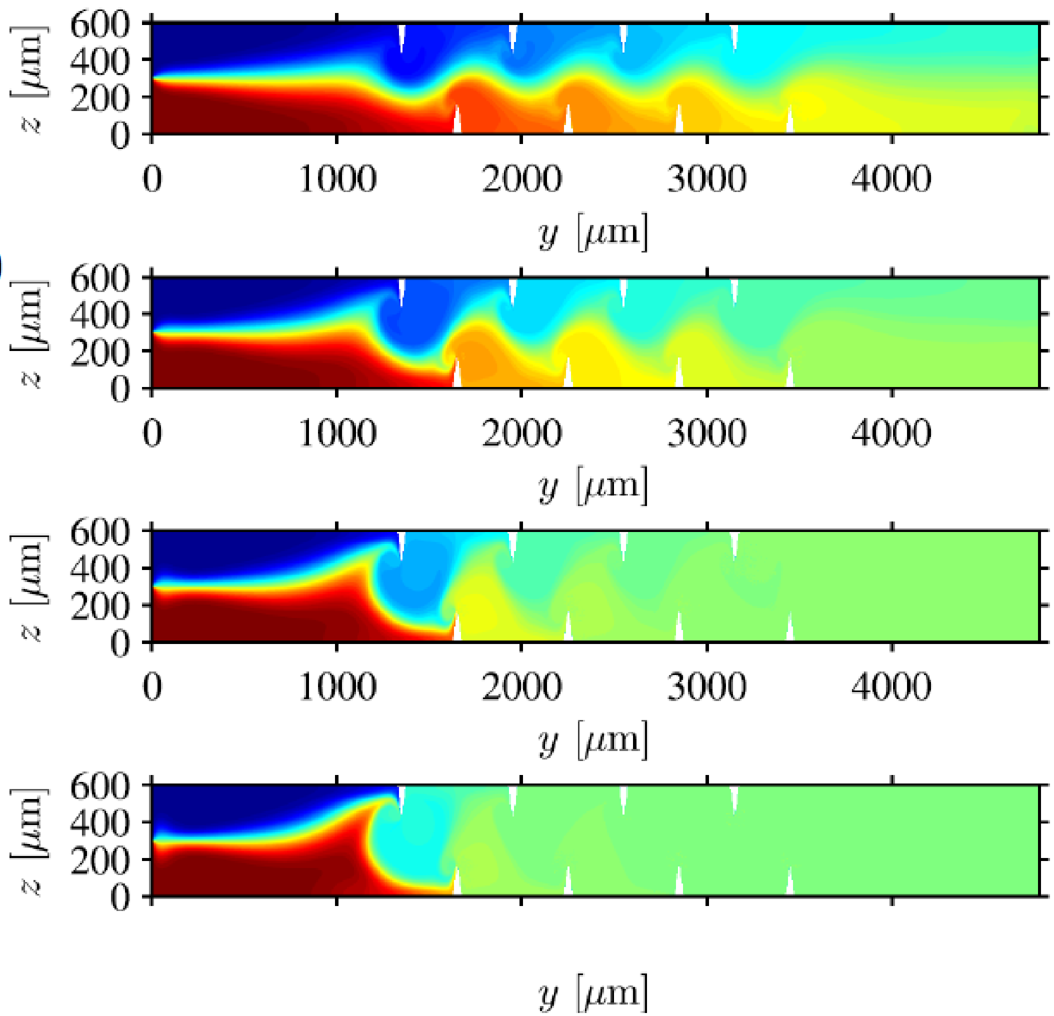


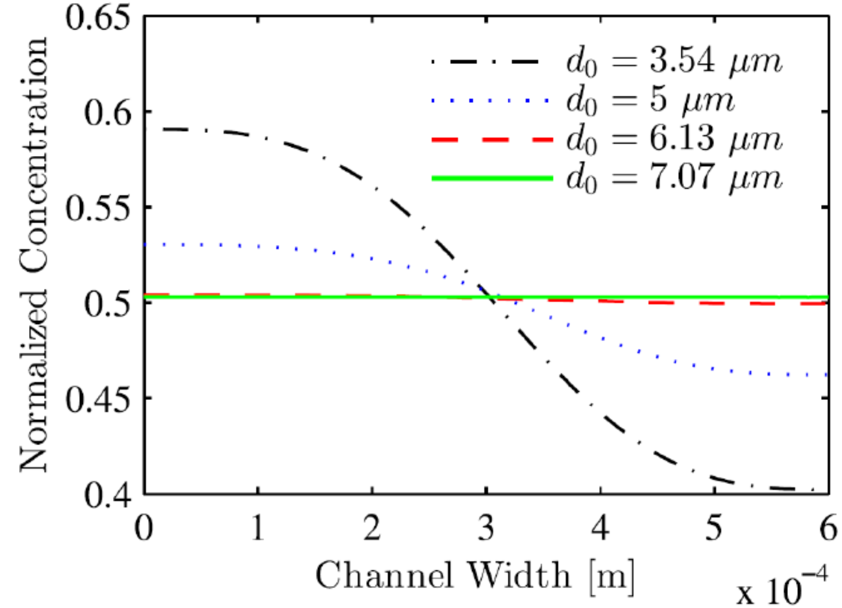
CONCENTRATION PROFILE





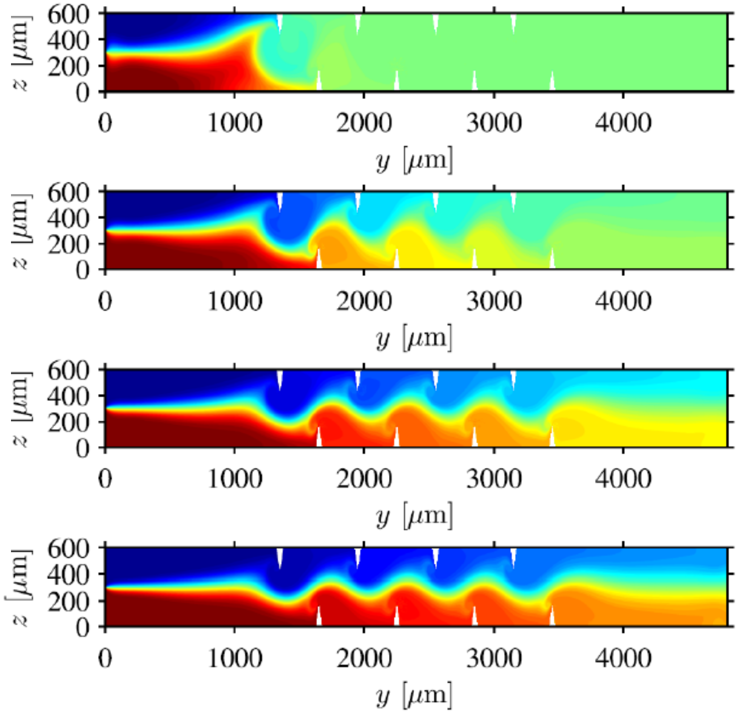
Effect of the applied power

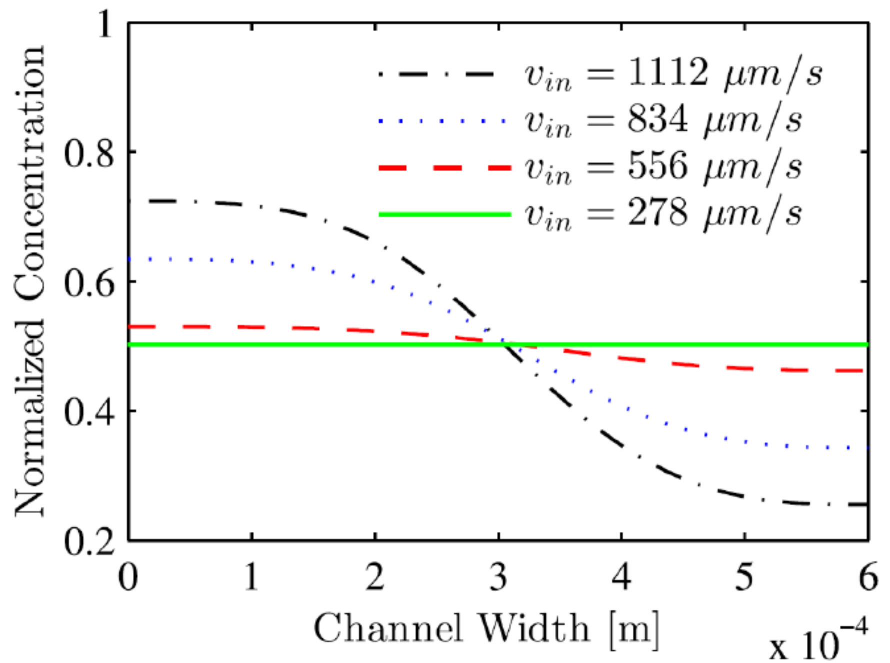




- High power => Faster mixing length => Ability to increase throughput for a desired mixing length

Effect of the inlet velocity





Second-Order Equations

$$\left\langle \frac{\partial \rho_2}{\partial t} \right\rangle + \nabla\cdot(\langle \rho_0 \mathbf{v}_2\rangle + \langle \rho_2 \mathbf{v}_0\rangle) = -\nabla\cdot\langle \rho_1 \mathbf{v}_1\rangle,$$

$$\begin{aligned} &\left\langle \rho_0 \frac{\partial \mathbf{v}_2}{\partial t}\right\rangle + \left\langle \rho_2 \frac{\partial \mathbf{v}_0}{\partial t}\right\rangle + \left\langle \rho_1 \frac{\partial \mathbf{v}_1}{\partial t}\right\rangle + \langle \rho_0 \mathbf{v}_1\cdot\nabla \mathbf{v}_1\rangle \\ &+ \langle \rho_0 \mathbf{v}_0\cdot\nabla \mathbf{v}_2\rangle + \langle \rho_0 \mathbf{v}_2\cdot\nabla \mathbf{v}_0\rangle + \langle \rho_1 \mathbf{v}_0\cdot\nabla \mathbf{v}_1\rangle \\ &+ \langle \rho_1 \mathbf{v}_1\cdot\nabla \mathbf{v}_0\rangle + \langle \rho_2 \mathbf{v}_0\cdot\nabla \mathbf{v}_0\rangle \\ &= -\nabla\langle p_2\rangle + \mu\nabla^2\langle \mathbf{v}_2\rangle + (\mu_b + \tfrac{1}{3}\mu)\nabla(\nabla\cdot\langle \mathbf{v}_2\rangle) \end{aligned}$$

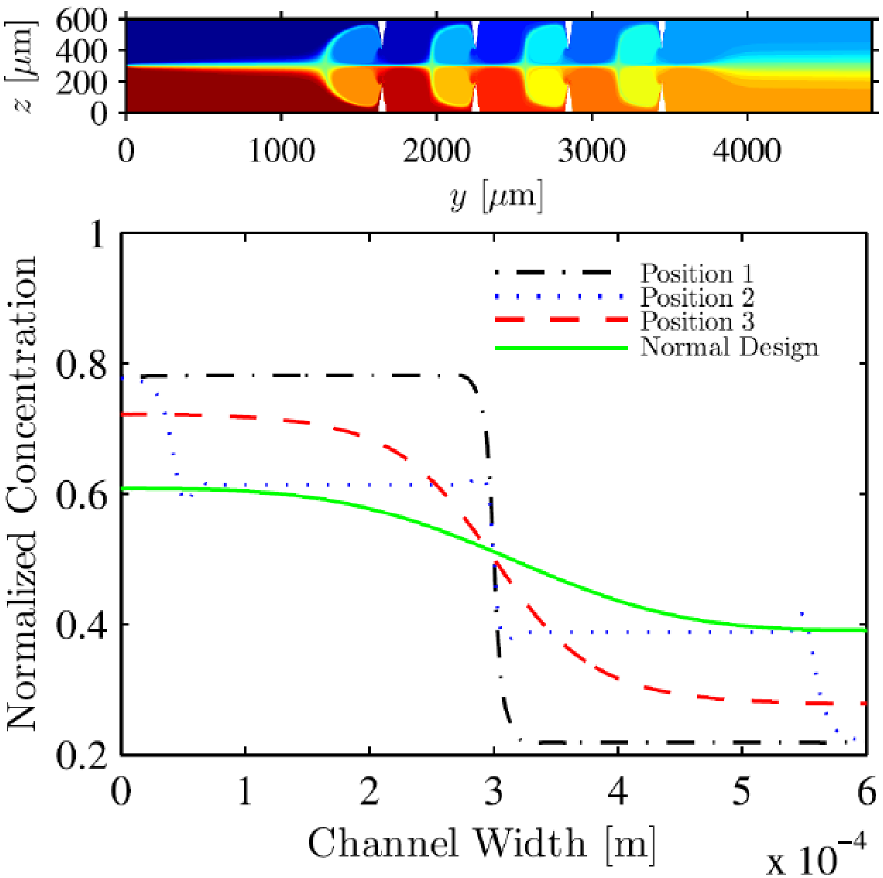
Effective convection velocity

$$\mathbf{v}^{C} = \mathbf{v}_0 + \mathbf{v}^{L}$$

- A change in inlet velocity has an effect on both the background flow as well as the streaming flow (due to some time-averaged terms containing inlet velocity).

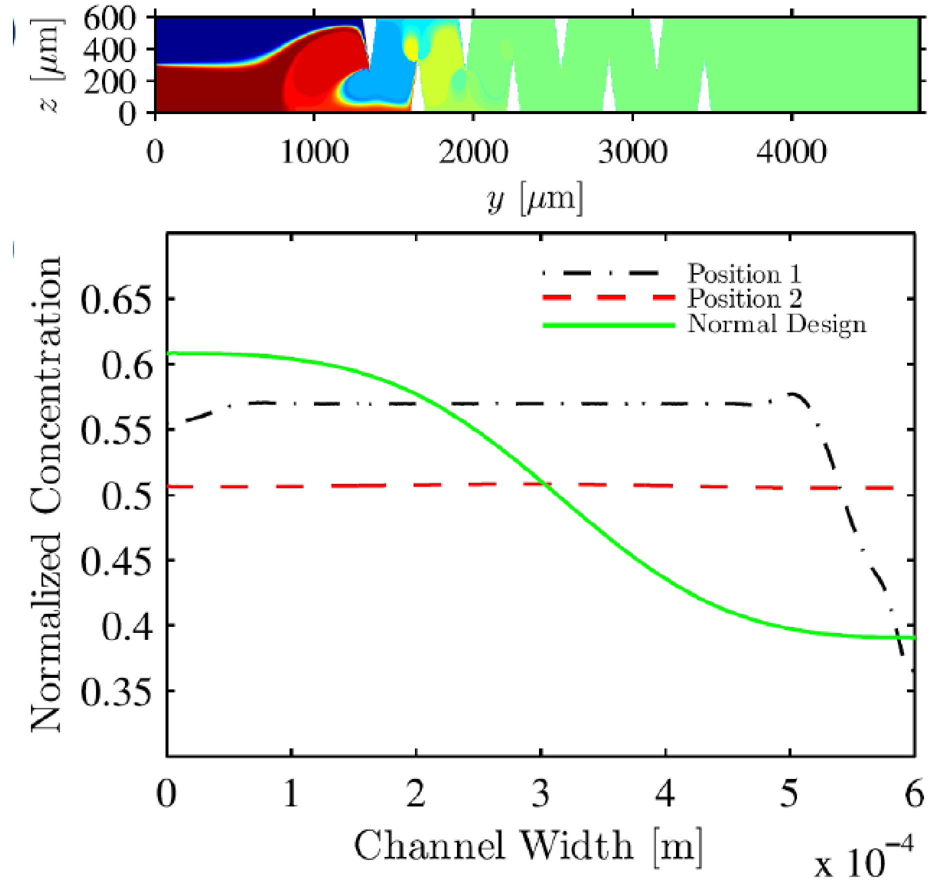
Different Designs

Opposite Sharp-Edges



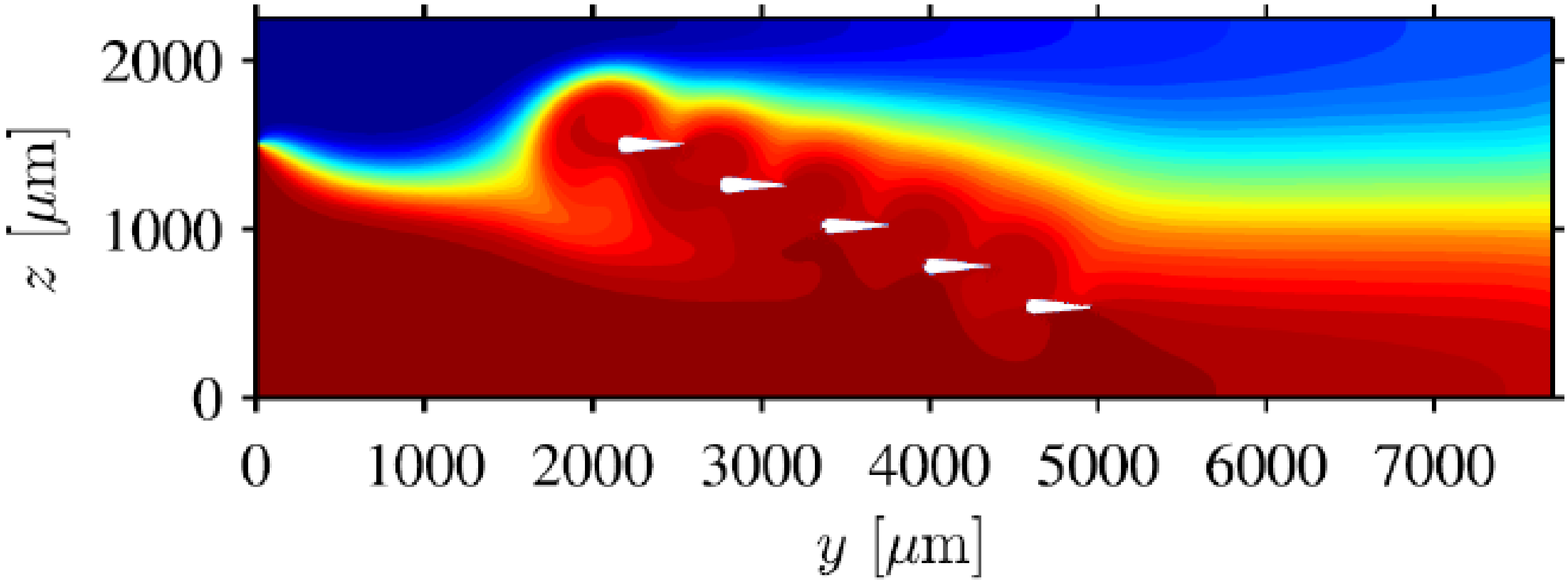
Streaming from the opposite edges suppresses each other.

Larger Sharp-Edges



Larger edges effectively perturbs both the incoming streams.

Concentration gradient



- The gradient profile can be spatially controlled by changing the arrangement of the sharp-edged structures.
- The gradient profile can be temporally controlled by tuning the inlet velocity or/and the applied power.
- Useful for studying temporal dynamics of cells in a chemical environment.

Conclusion and Outlook

- A numerical model for sharp-edge based mixing is presented with good qualitatively comparison with the experiments.
- The effects of operational and geometrical parameters was investigated.
- The exact displacement profile at the walls need to be further investigated.
- Quantitative 3D Astigmatism Particle Tracking Velocimetry (APTV) measurements for the experimental verification are in progress.

Acknowledgments

Po-Hsun Huang | **Tony Jun Huang** | **Francesco Costanzo**

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