# Geometric Optimization of Micromixers

COMSOL CONFERENCE BOSTON

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#### Introduction

- > Micromixing is a key step in realizing fast analysis time in many bio-chemical, biological and detection applications of Lab-on-a-chip (LOC) devices.
- > The conventional T-mixer design requires longer channel lengths and times to achieve complete mixing owing to its dependence on transverse diffusion.
- > In this work, we investigate the effect of pattern/ groove shape on mixing performance. The geometric optimization is carried out for:
- (a) Heterogeneous charge bottom electro-kinetic micromixer and;
- (b) Pressure driven flow based groove micromixer.

#### **Mathematical Model**

Navier Stokes equation and Continuity equation is solved for obtaining pressure and velocity field.

$$\rho(u \cdot \nabla u) = -\nabla p + \mu \nabla^2 u$$
$$\nabla \cdot u = 0$$

> Convection- Diffusion equation

$$(u \cdot \nabla c) = D\nabla^2 c$$

> Electroosmotic flow (EOF) is modeled using the following additional equations; Laplace equation is solved for potential distribution.

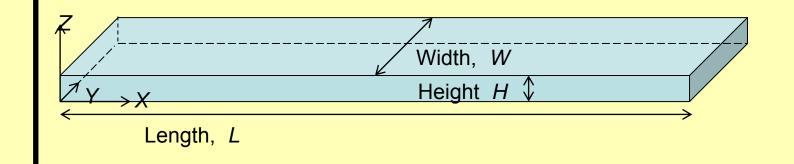
$$\nabla^2 \psi = 0; \quad E = -\nabla \psi$$

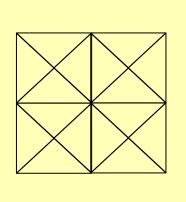
Smoluchowski's slip velocity condition is used with an assumption of thin electric double layer (EDL).

$$u_{slip} \sim -\frac{\varepsilon_m \varsigma}{\mu} E$$

#### Methodology COMSOL solves the governing equations (flow, mass transport and electric potential distribution) for the initial geometry/pattern. Using the concentration field compute the mixing index $\eta$ . Pass (I, $\eta$ ) to MATLAB optimizer MATLAB determines if COMSOL solves FEM mode optimum η has been reached. If not searches the space of I shape/boundary conditions and returns η<sup>p+1</sup> for the best guess optimum Comsol 3.5a & Matlab

### Design of Optimal Heterogeneous Charge Pattern using Binary Optimization

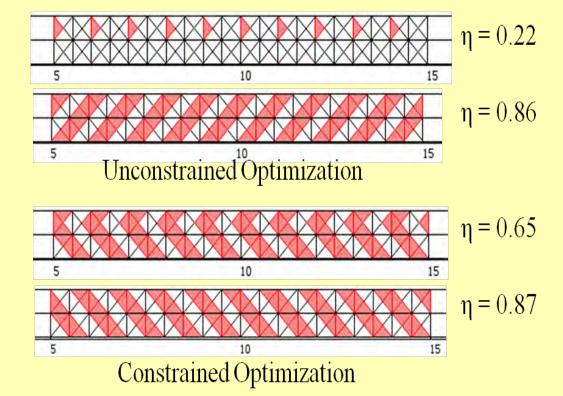




Heterogeneous charge pattern is represented by 10 unit blocks from x = 5-15. A unit block consists of 16 triangular elements; as shown on the left.

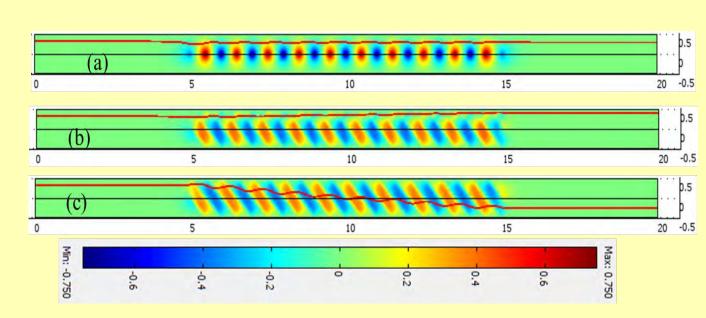
Surface charge on each triangular patch  $(S_i)$ in unit block is treated as a binary variable,

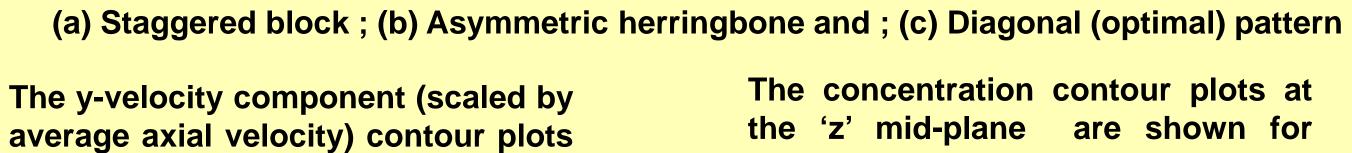
$$S_i = \begin{cases} 0 \\ 1 \end{cases}$$



This discretization approach is capable of generating 2<sup>16</sup> design patterns.

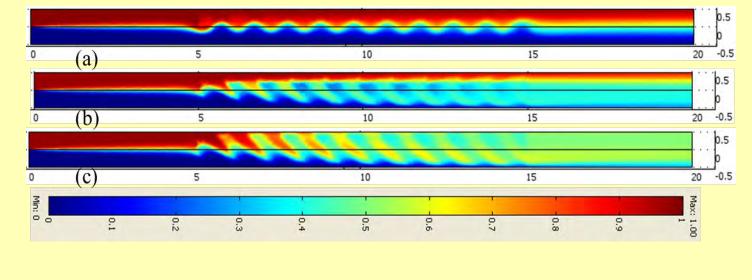
diagonal heterogeneous charge pattern found to provide the best mixing performance for both unconstrained as well as constrained optimization case.





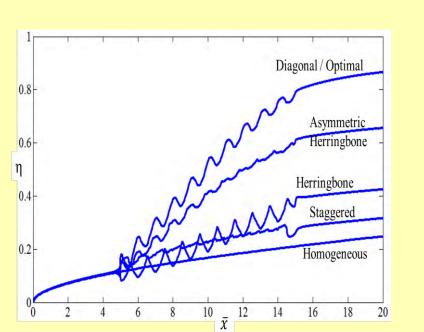
The diagonal patterns generate alternate bands of positive and negative y-velocity across the entire channel width which results in

at the 'z' mid-plane are shown.



The concentration contour plots at the 'z' mid-plane are shown for various pattern designs.

The diagonal heterogeneous charge pattern generates the most favorable transverse flow structure to provide superior mixing performance with = 0.87 at Re ~ 0.1 and Pe ~ 1075.

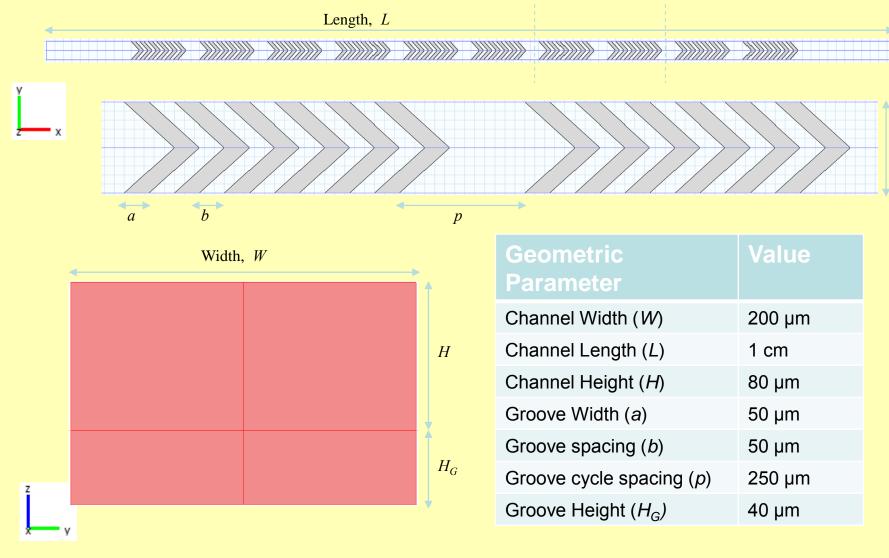


(2010b) is used.

The axial mixing index plot for various designs is shown above. The optimal design provides more than three-fold improvement in mixing performance w.r.t" the homogeneous T-mixer"

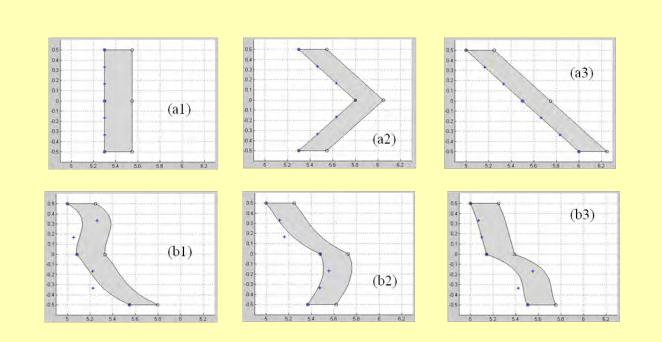
### Design of Optimal Groove Structure using Bézier Curve Approach

improved mixing performance.



A total of 60 grooves are axially distributed in form of 10 groove cycles containing 6 grooves per cycle.

The effect of groove shape on mixing performance is studied; a single groove shape is optimized and same shape is applied to all the grooves in the channel.

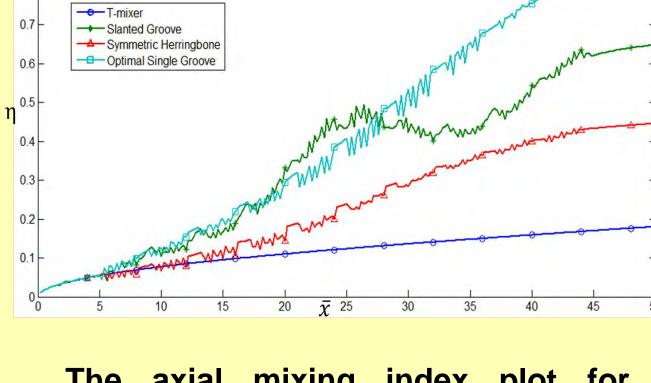


The groove shape is parametrically represented by the Bézier curve, P(t).

$$P(t) = \sum_{i=0}^{n} B_i J_{n,i}(t) \qquad 0 \le t \le 1$$

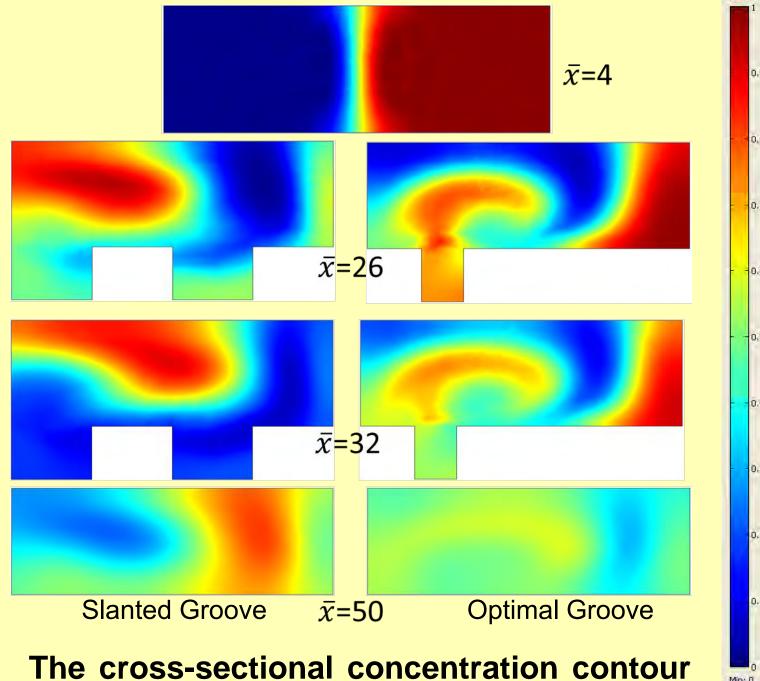
$$J_{n,i}(t) = \frac{n!}{i! (n-i)!} t^i (1-t)^{n-i}$$

The optimal groove shape as identified by the optimization approach.



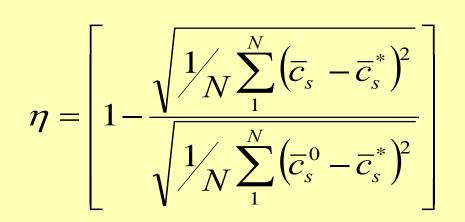
The axial mixing index plot for various groove designs is shown above.

groove structure favorable generates the most transverse flow structure to provide superior mixing performance with = 0.85 at Pe  $\sim 4200$ .

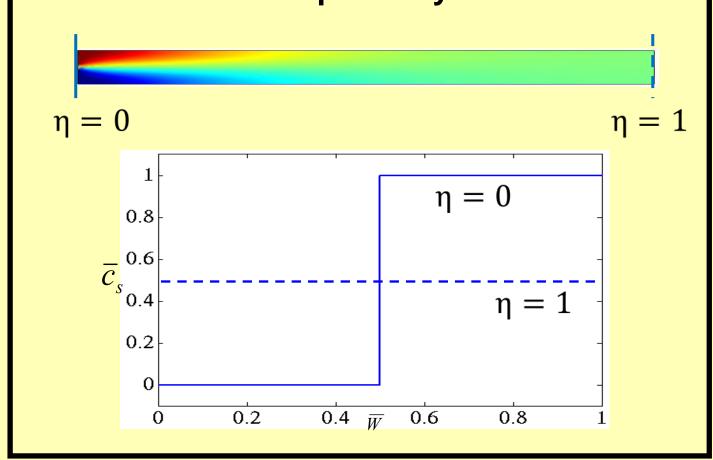


plots are shown at various axial locations for SGM and optimal groove designs.

## Mixing Index

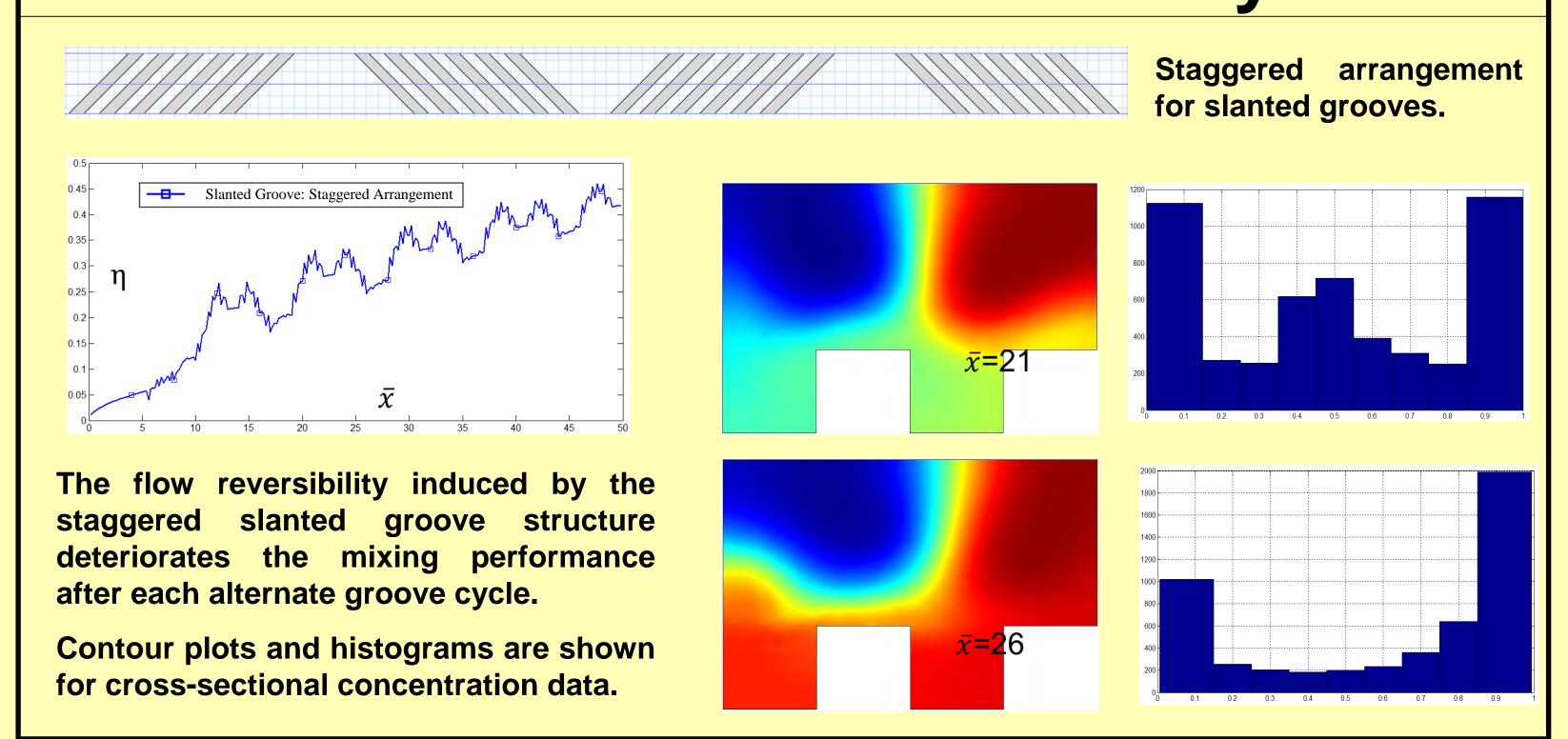


Mixing index is based on the standard deviation from the perfectly mixed state.



### Effect of Flow Reversibility

Optimal Groove



#### Conclusions

- > Binary optimization is utilized to identify the optimal heterogeneous charge pattern for improved electrokinetic micromixing.
- Bezier curve based approach is employed for groove shape optimization for pressure driven flow based groove micromixers.
- > The proposed approach could be utilized for microdevice design optimization.

#### References

- Nguyen, N. T., & Wu, Z. G. (2005). Micromixers A Review, Journal of Micromechanics and Microengineering, 15(2), R1-R16. Stroock, A. D., et. al. (2002). Chaotic Mixer for Microchannels, Science,
- 25;295(5555):647-51. Jain, M., & Nandakumar, K. (2012). Optimal Patterning of Heterogeneous Surface Charge for Improved Electrokinetic
- Micromixing, accepted for publication in Comp & Chem. Engg. Jain, M., Rao, A. & Nandakumar, K. (2012). Numerical Study on Shape Optimization of Groove Micromixers, submitted to Microfluidics and Nanofluidics.