COMSOL CONFERENCE BOSTON 2012

PRESENTATION

Study on Groove Shape Optimization for Micromixers

M. Jain, Abhijit Rao and K. Nandakumar

Cain Dept. of Chemical Engineering,

Louisiana State University

Comsol Conference 2012, Boston.

Outline

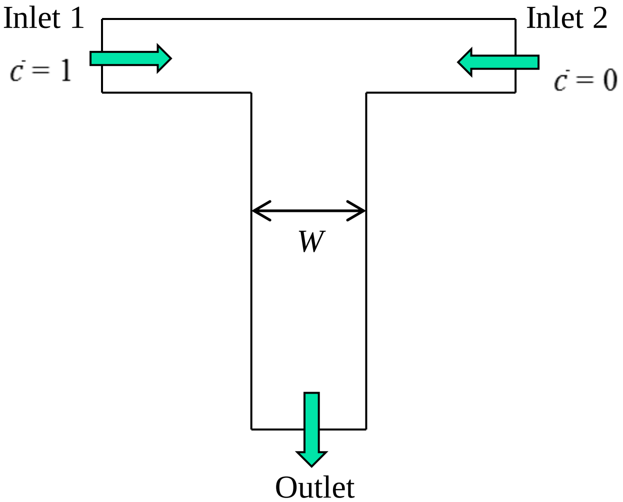
- Introduction to Micromixing
- Floor Groove Micromixers (SGM, SHM)
- Modeling & Shape Optimization Approach
- Optimization Results & Parametric Studies
- Conclusions

Micromixing

Two main applications for micromixing are:

(a) Lab-on-a-Chip applications (dilution, biochemical reaction and detection, enzyme assays etc.)

(b) Micro-reactor based chemical synthesis (microscopic length scale favors heat transfer and allows better control of chemical reactions).



The most basic micromixer is a T-mixer where two confluent streams mix due to molecular diffusion.

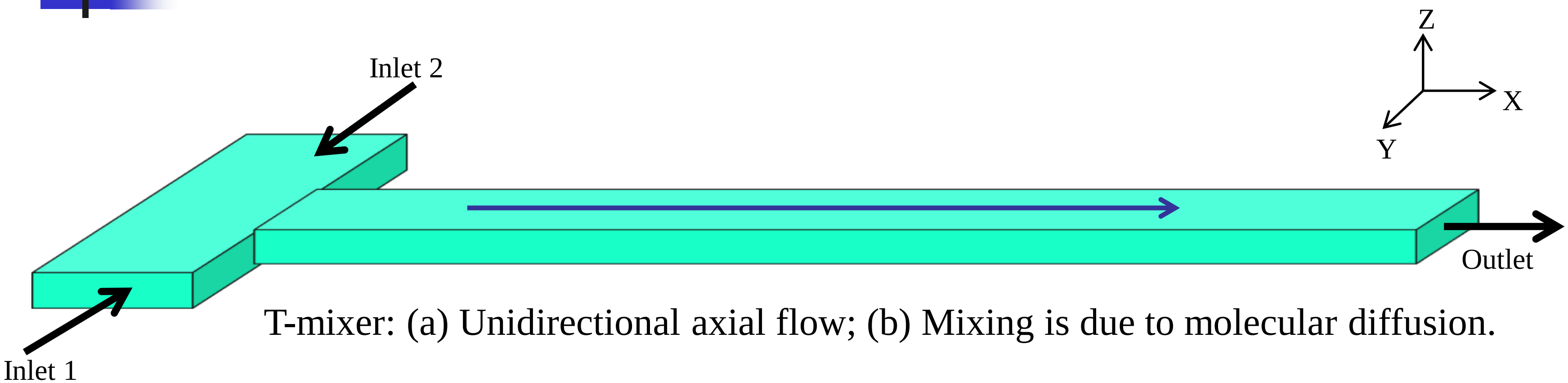
$$\tau_d \sim \frac{{l_d}^2}{D} = \frac{W^2}{D} \qquad L_m \sim \frac{UW^2}{D} = Pe \cdot W$$

Enhancing Micromixing

Micromixing could be enhanced by reduction in effective diffusion length and/or by increase in interfacial surface area. Some of the reported techniques for parallel flow type micromixers are:

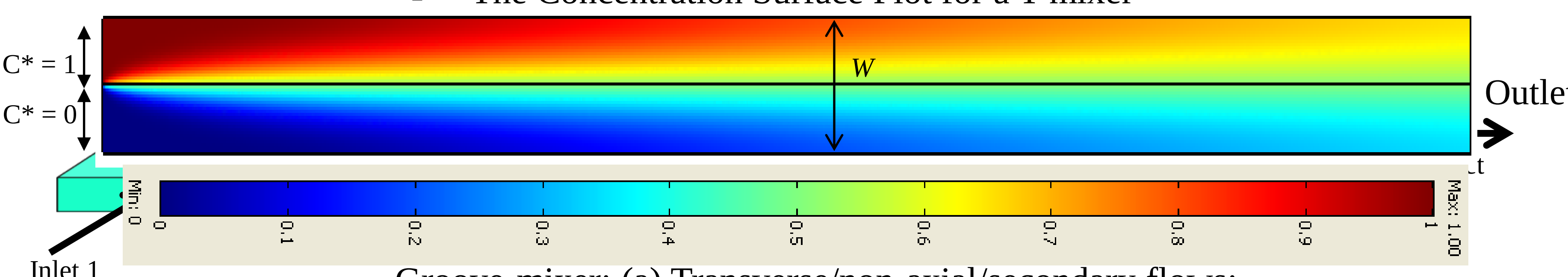
- Lamination of multiple input streams
- Flow focusing using sheath flow
- Geometric modification to induce transverse flows (groove/ribs) on the channel bottom, physical constrictions etc.
- Heterogeneous surface charge on channel bottom or sidewalls for electrokinetic micromixing
- External disturbances (pressure, electrokinetic) to induce transverse flows

Floor Groove Micromixers



T-mixer: (a) Unidirectional axial flow; (b) Mixing is due to molecular diffusion.

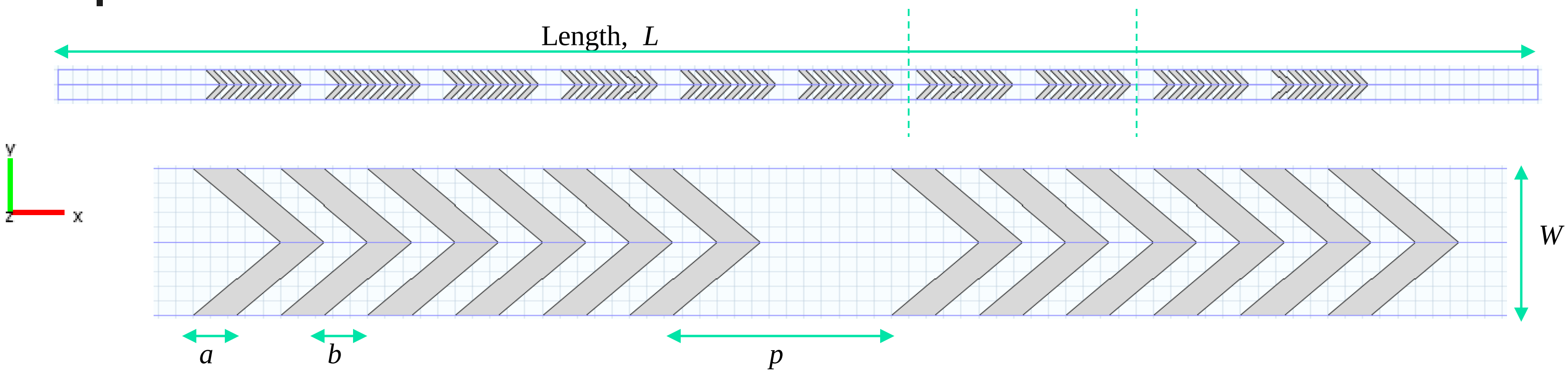
The Concentration Surface Plot for a T-mixer

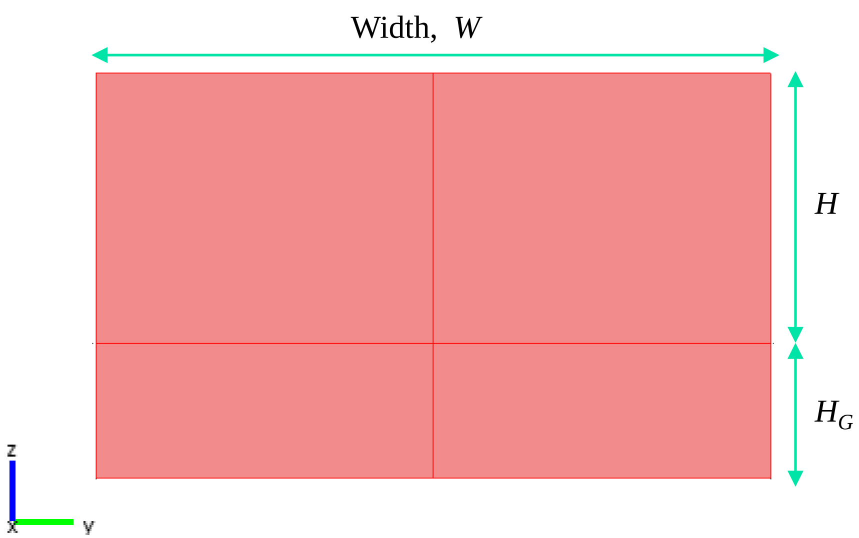


Groove-mixer: (a) Transverse/non-axial/secondary flows;
(b) Mixing performance is improved due to advection.

Stroock A. D., Dertinger S. K. W., Ajdari A., Mezic I., Stone H. A., and Whitesides G. M., Chaotic Mixer for Microchannels, Science, 25, 647-51, (2002).
Johnson T.J, Ross D., and Locascio L.E., Rapid microfluidic mixing, Anal Chem, 74(1), 45-51, (2002).

Geometric Details





Geometric Parameter	Value
Channel Width (*W*)	200 µm
Channel Length (*L*)	1 cm
Channel Height (*H*)	80 µm
Groove Width (*a*)	50 µm
Groove spacing (*b*)	50 µm
Groove cycle spacing (*p*)	250 µm
Groove Height (H_G)	40 µm

Modeling Groove Micromixers

$$L_{\mathrm{ref}} = W, \quad c_{\mathrm{ref}} = c_{0,} \quad u_{\mathrm{ref}} = u_{av} = \frac{Q}{WH}, \quad p_{ref} = \frac{\mu\, u_{av}}{W}, \text{and}$$

$$\bar{x} = \frac{x}{L_{\mathrm{ref}}}, \quad \bar{y} = \frac{y}{L_{\mathrm{ref}}}, \quad \bar{z} = \frac{z}{L_{\mathrm{ref}}}, \quad \bar{u} = \frac{u}{u_{\mathrm{ref}}}, \quad \bar{v} = \frac{v}{u_{\mathrm{ref}}}, \quad \bar{w} = \frac{w}{u_{\mathrm{ref}}}, \quad \bar{p} = \frac{p}{p_{\mathrm{ref}}}$$

Navier Stokes & Continuity equation

$$Re(\bar{u} \cdot \bar{\nabla} \bar{u}) = -\bar{\nabla} \bar{p} + \bar{\nabla}^2 \bar{u} \longrightarrow$$

$$\bar{\nabla} \cdot \bar{u} = 0$$

Convection-Diffusion Equation

$$Pe\,(\bar{u} \cdot \bar{\nabla} \bar{c}_s) = \bar{\nabla}^2 \bar{c}_s \longrightarrow$$

The mixing performance or efficiency is estimated using the concentration field.

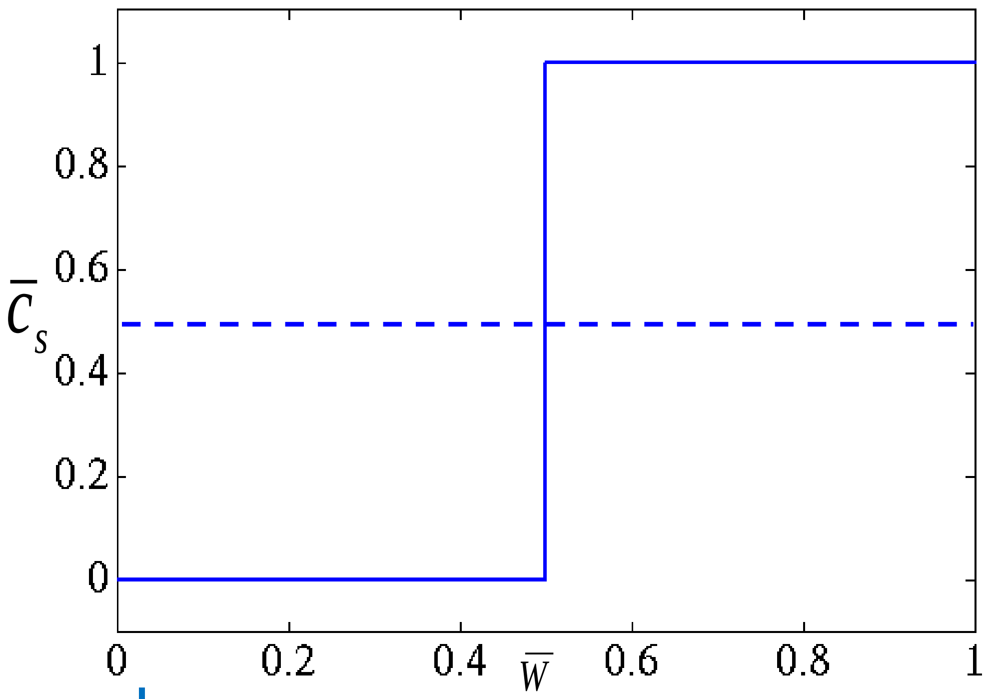
Reynolds Number

$$Re = \frac{\rho\, u_{av}\, L_{ref}}{\mu}$$

Peclet Number

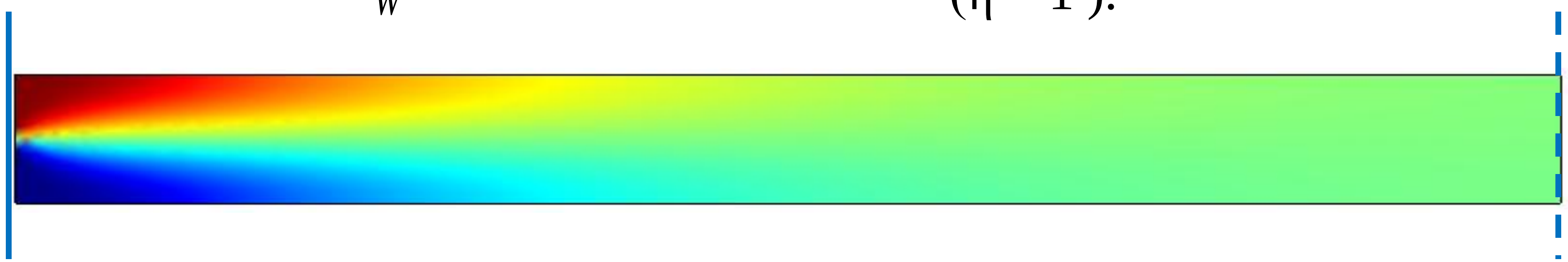
$$Pe = \frac{u_{ref} L_{ref}}{D} = \frac{Q}{HD}$$

Mixing Performance Index

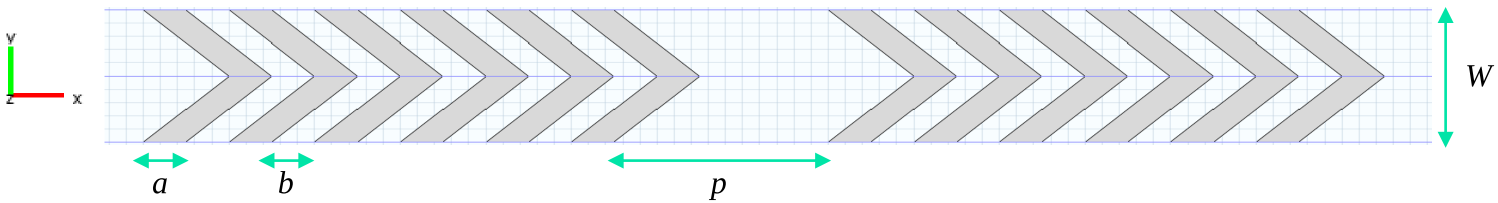


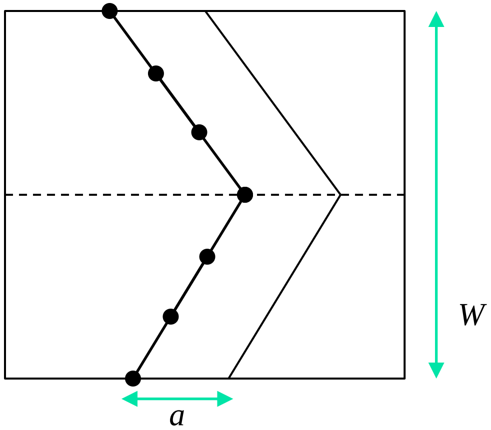
$$\eta = \left[1 - \frac{\sqrt{\frac{1}{N}\sum_{1}^{N}\left(\bar{c}_s - \bar{c}_s^{*}\right)^2}}{\sqrt{\frac{1}{N}\sum_{1}^{N}\left(\bar{c}_s^{0} - \bar{c}_s^{*}\right)^2}} \right]$$

The solid line corresponds to perfectly unmixed state (η = 0, inlet condition for parallel flow mixer). The dashed line represents perfectly mixed state (η = 1).



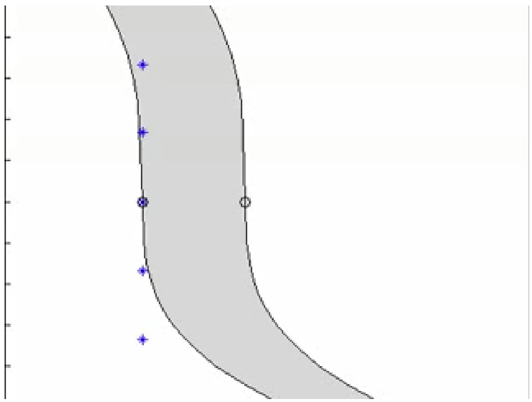
Optimization Approach

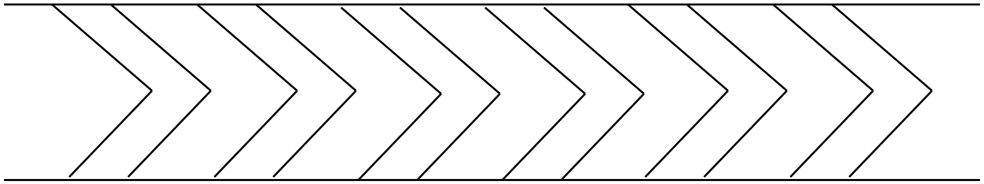




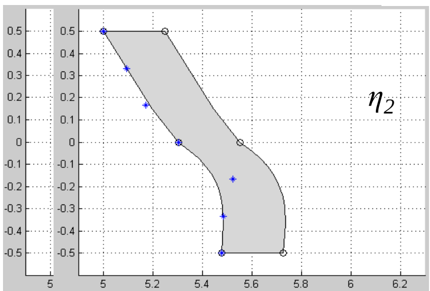
$$P(t) = \sum_{i=0}^{n} B_i J_{n,i}(t) \qquad 0 \le t \le 1$$

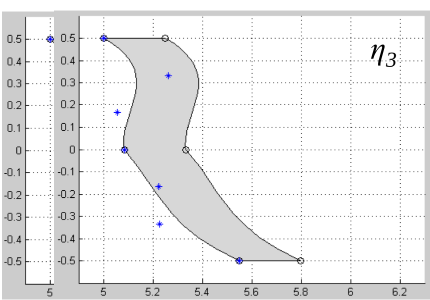
$$J_{n,i}(t) = \frac{n!}{i!\,(n-i)!} t^i (1-t)^{n-i}$$

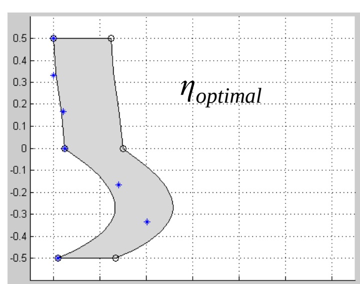




Optimization Implementation

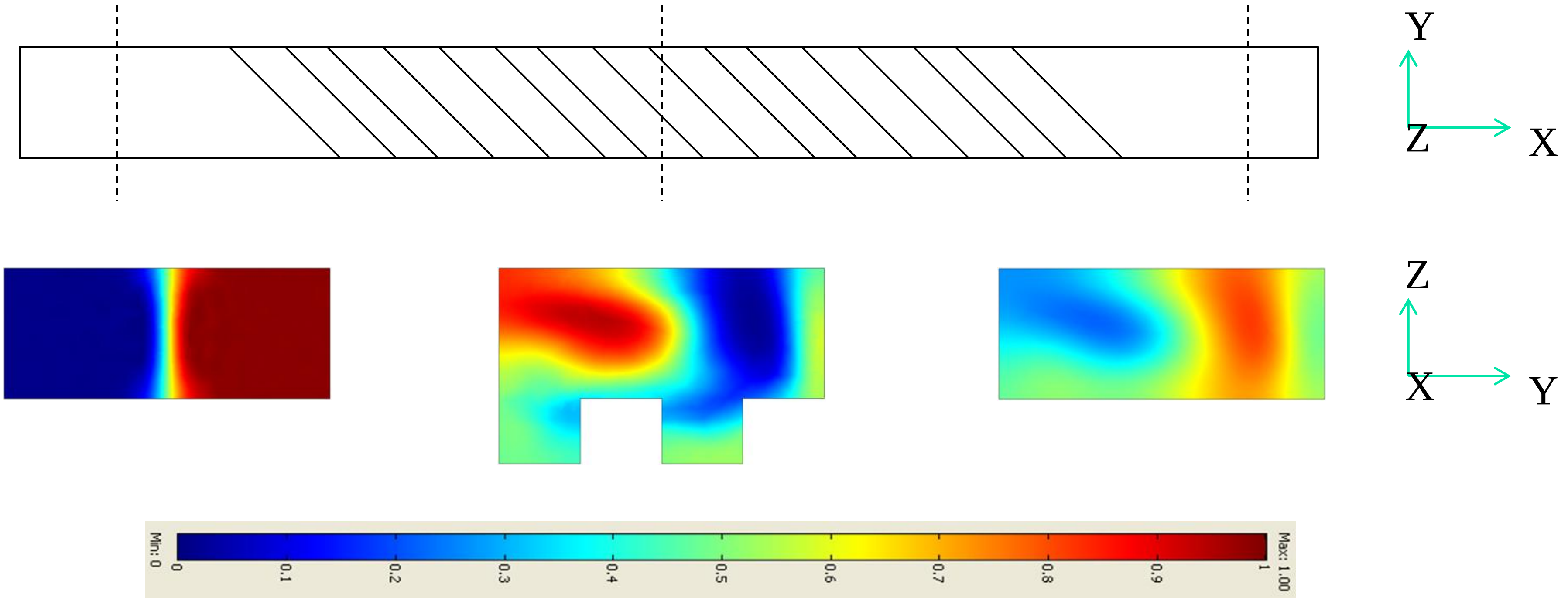






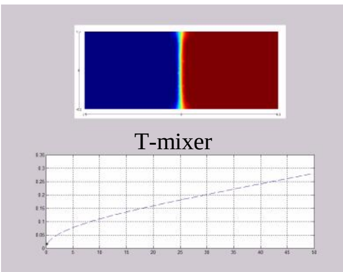
COMSOL solves the governing equations(flow and mass transport) for the initial groove structure.
Using the concentration field compute the mixing index η.
Pass (I, η) to MATLAB optimizer
(I^0, η^0)
MATLAB determines if optimum η has been reached. If not searches the space of I for the best guess
(η^{p+1})
COMSOL solves FEM model for I^{p+1} with new groove structure and returns η^{p+1}
(I^{p+1}, η^p)
Is η^p optimum ?
(I^{p+1})
No
Yes
Stop

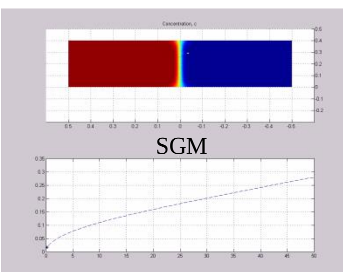
Single Groove Optimization

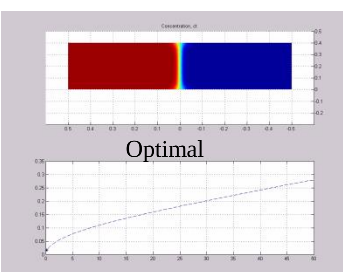


Optimization is carried out at $Q = 2\ \mu l/min$ (Pe ~4200, based on average axial velocity)

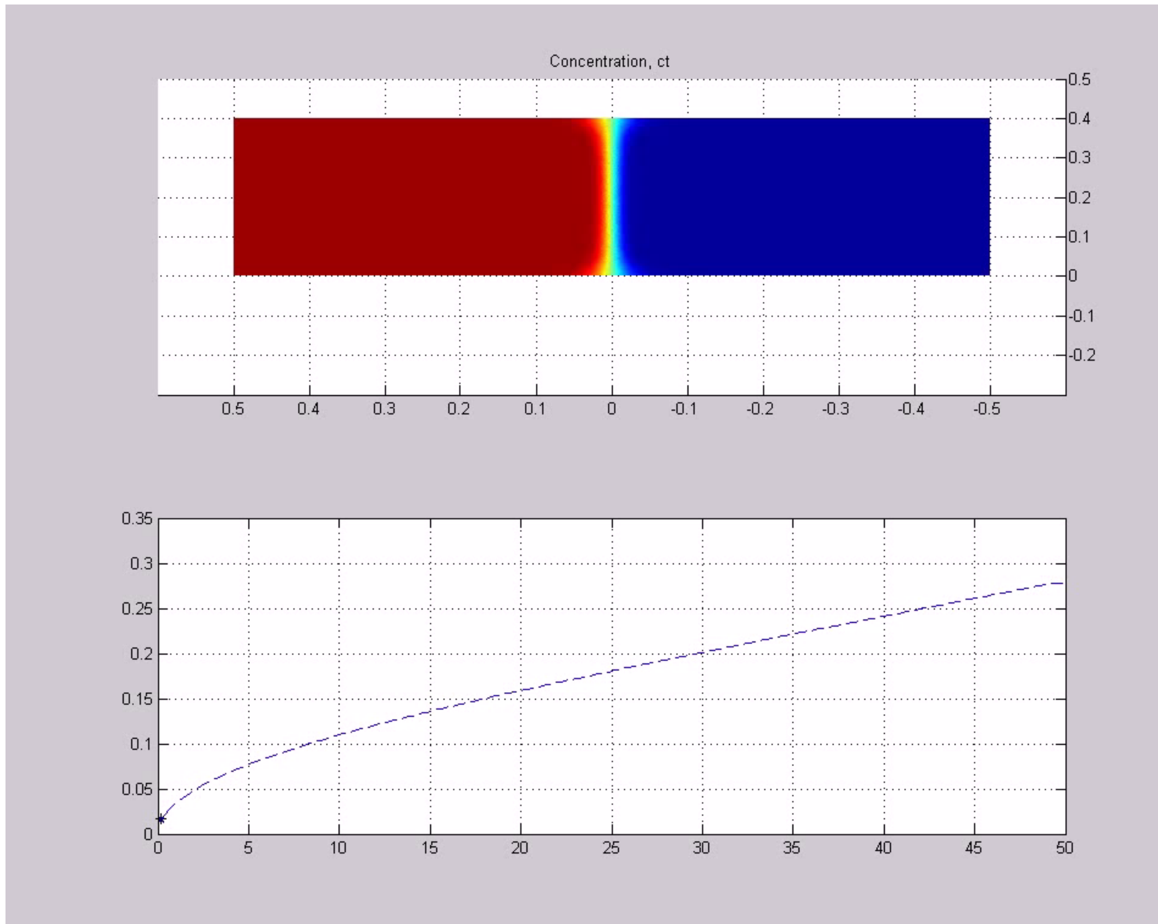
Single Groove Optimization



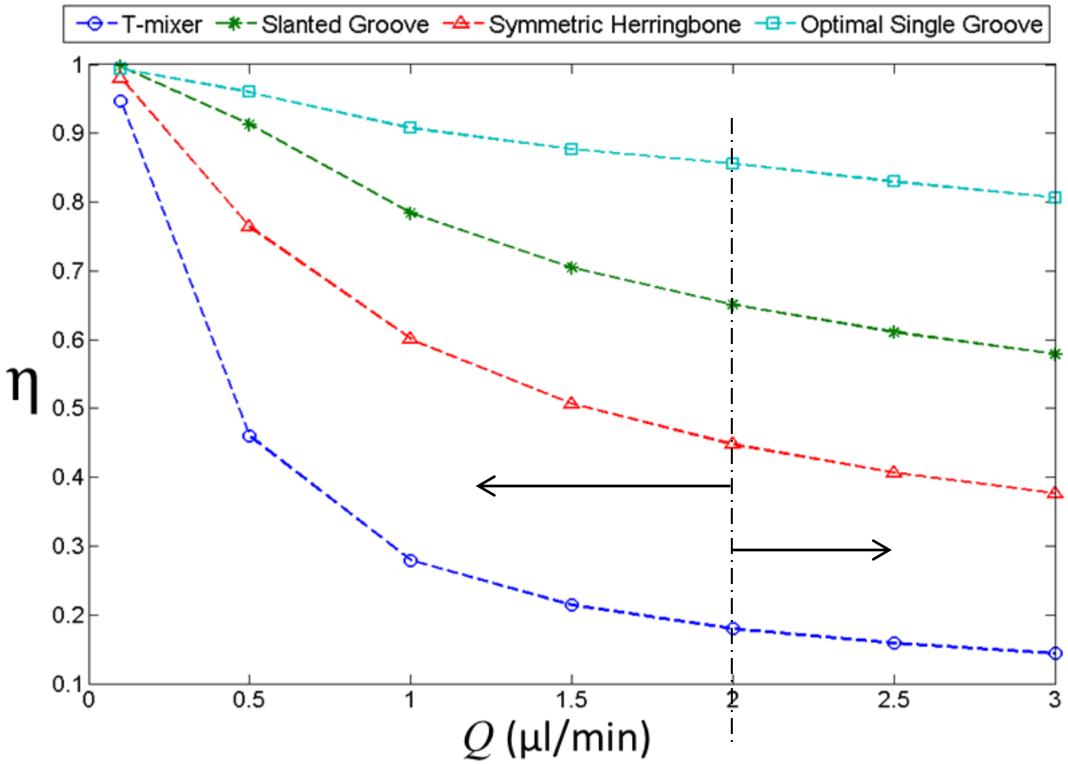




Optimal



Single Groove Optimization



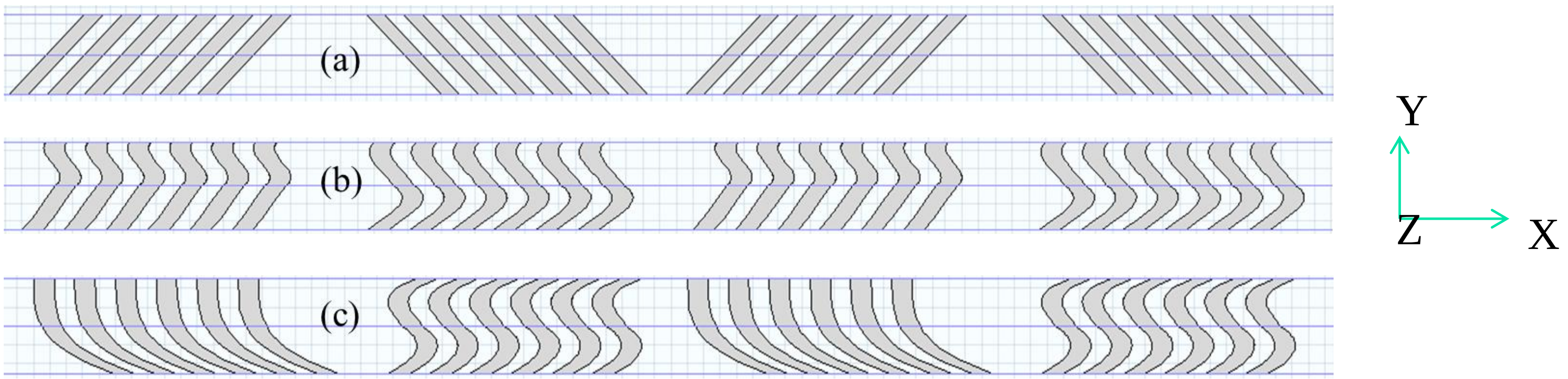
Optimal groove structure (identified at Q = 2 *μl/min*; Pe ~4200) provides superior mixing performance even at different Pe values/ flow rates.

COMSOL CONFERENCE BOSTON 2012

LSU LOUISIANA STATE UNIVERSITY

Staggered Groove Optimization

Shape optimization is studied for staggered groove arrangement by parametrically representing the first grooves of 1st and 2nd groove cycle as shown in figure below.

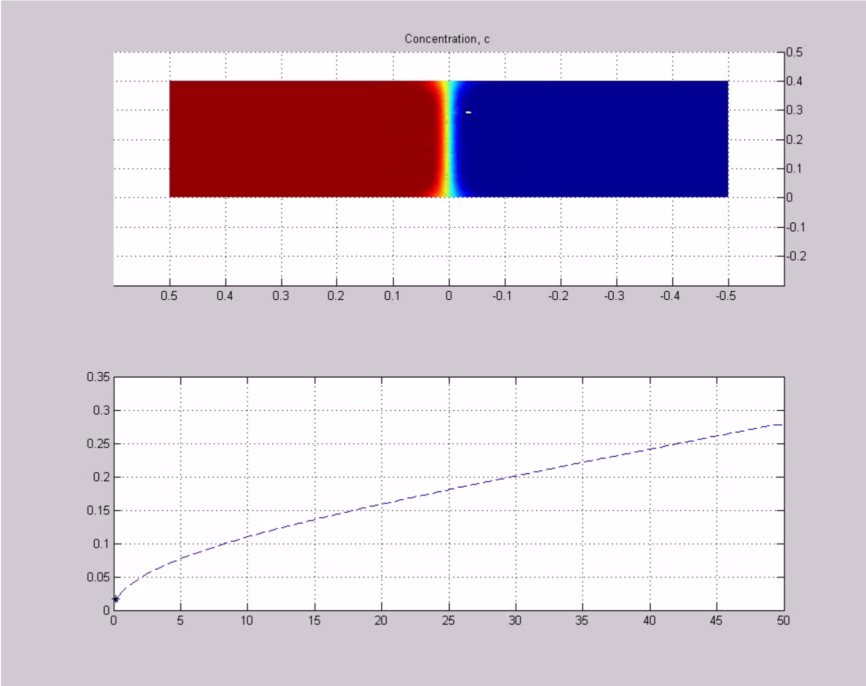


Staggered arrangement for (a) Slanted groove design; (b) Optimal staggered groove -1 (OSG-1) and; (c) Optimal staggered groove -2 (OSG-2).

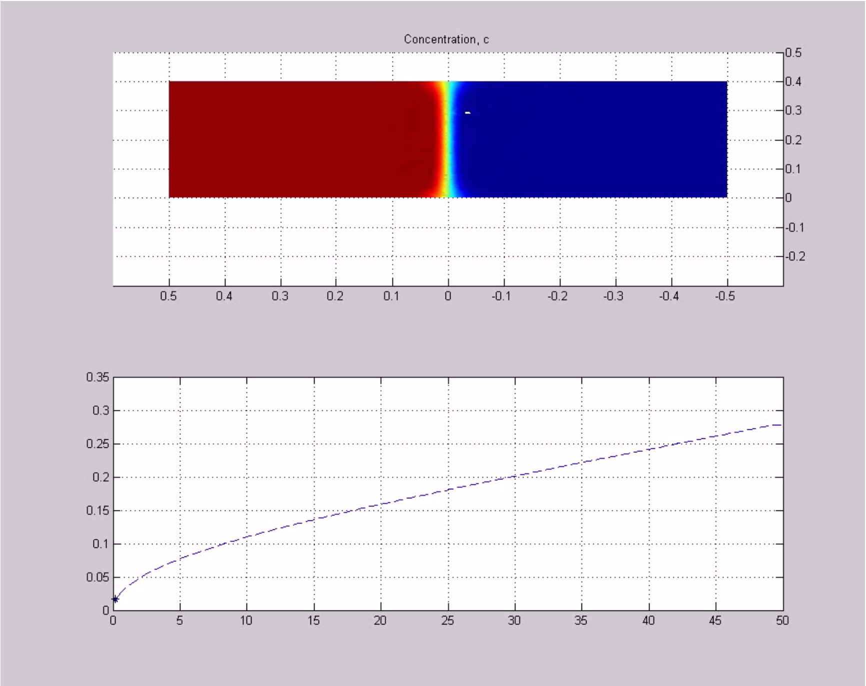
These optimal staggered designs are found using the same approach as used for the single groove optimization case.

Staggered Groove Optimization

SHM/ OSG-1



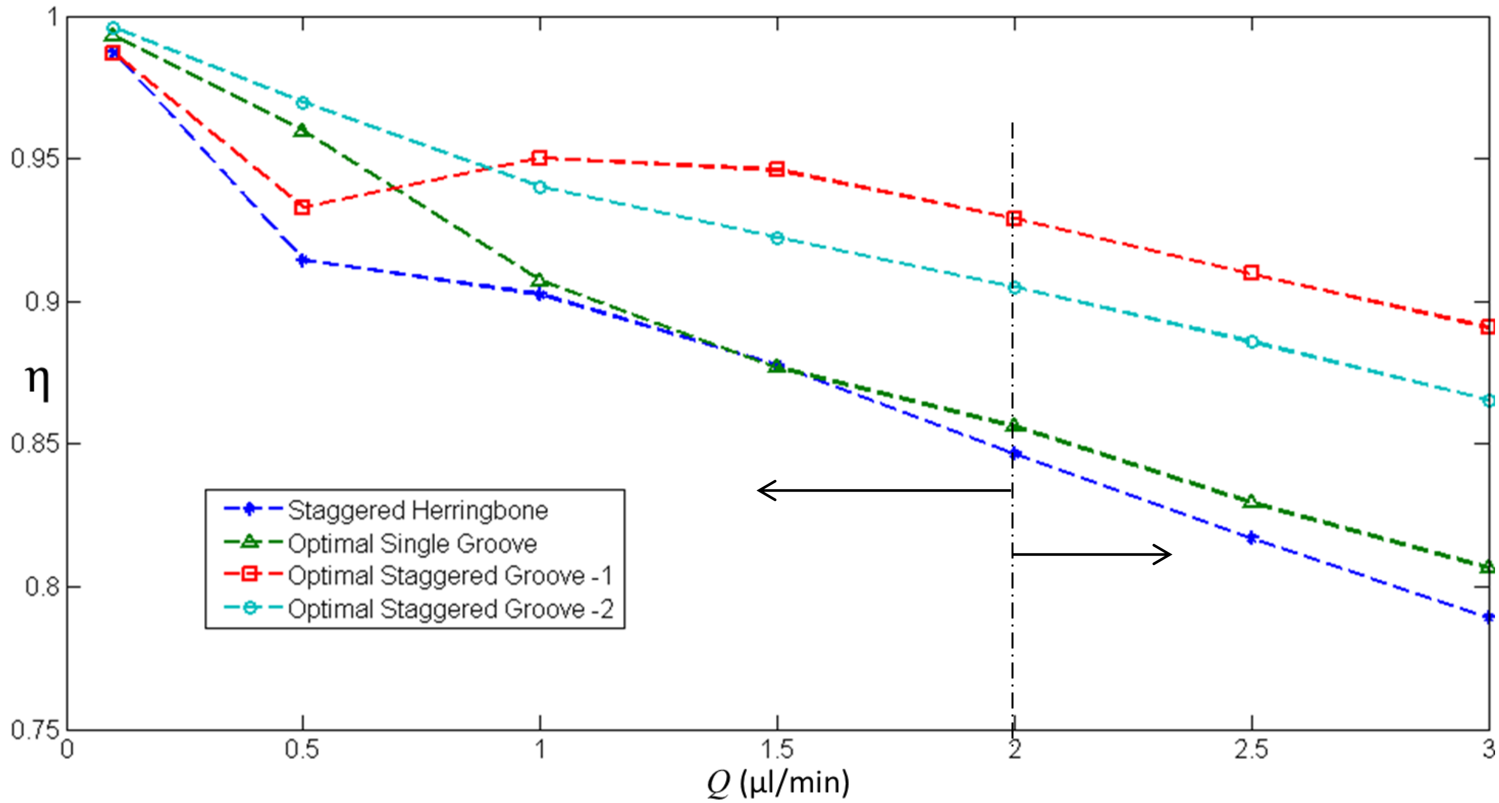
OSG-2



COMSOL CONFERENCE BOSTON 2012

LOUISIANA STATE UNIVERSITY

Staggered Groove Optimization



Optimal groove structures (OSG-1 & OSG-2, identified at Q = 2 $\mu l/min$; Pe ~4200) provides superior mixing performance even at different Pe values/ flow rates.

Conclusions

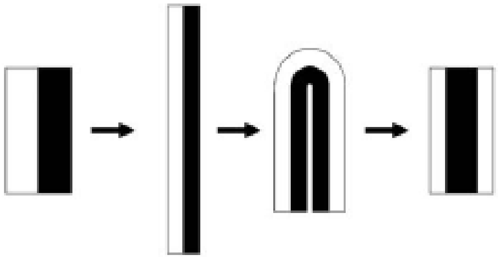
- The effect of groove shape on the mixing performance of groove micro mixers is analyzed.
- The optimal groove structure is obtained by employing parametric Bézier curve representation of the groove shape.
- The superior mixing performance of optimal design is due to the generated transverse flow which results in higher interfacial area for mass transfer.
- The optimal groove is parametrically compared with other groove types and found to provide the best mixing performance for a range of Pe numbers studied.

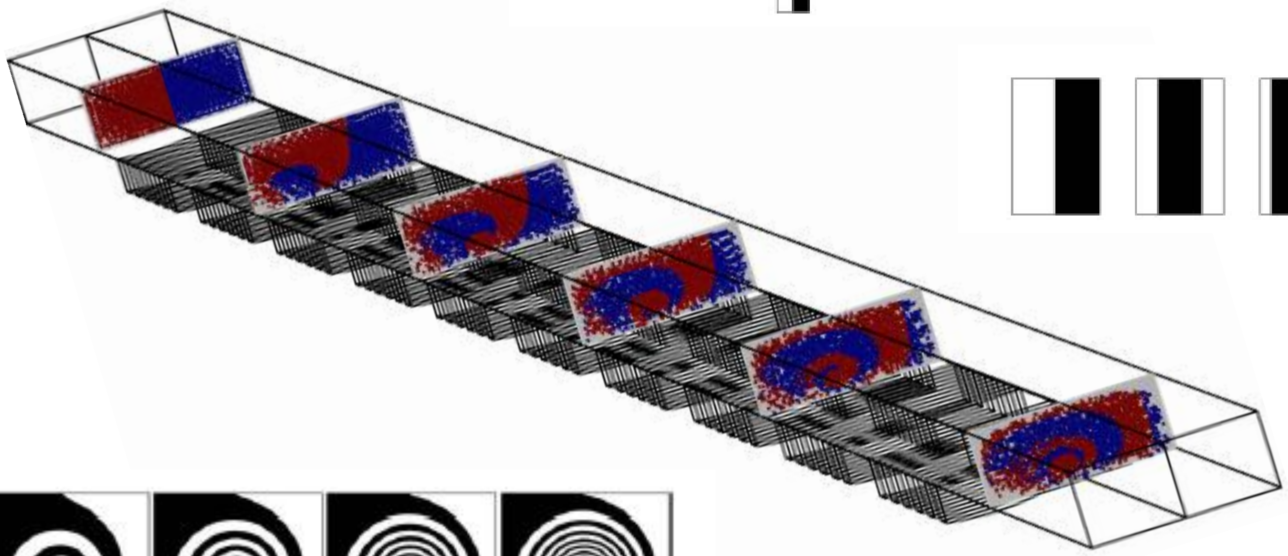
Acknowledgements

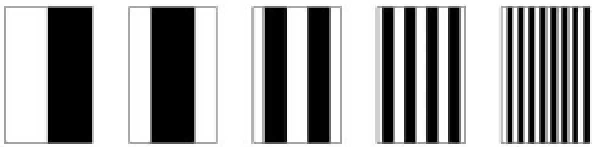
- Cain Chair Program at Chem. Engg. Dept., LSU
- Louisiana Optical Network Initiative (LONI)
- High Performance Computing (HPC) at LSU.
- Research Group Members.

Questions?

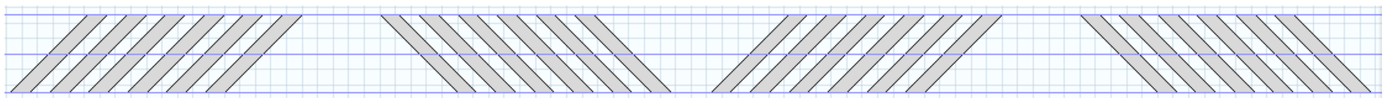
Chaotic Mixing

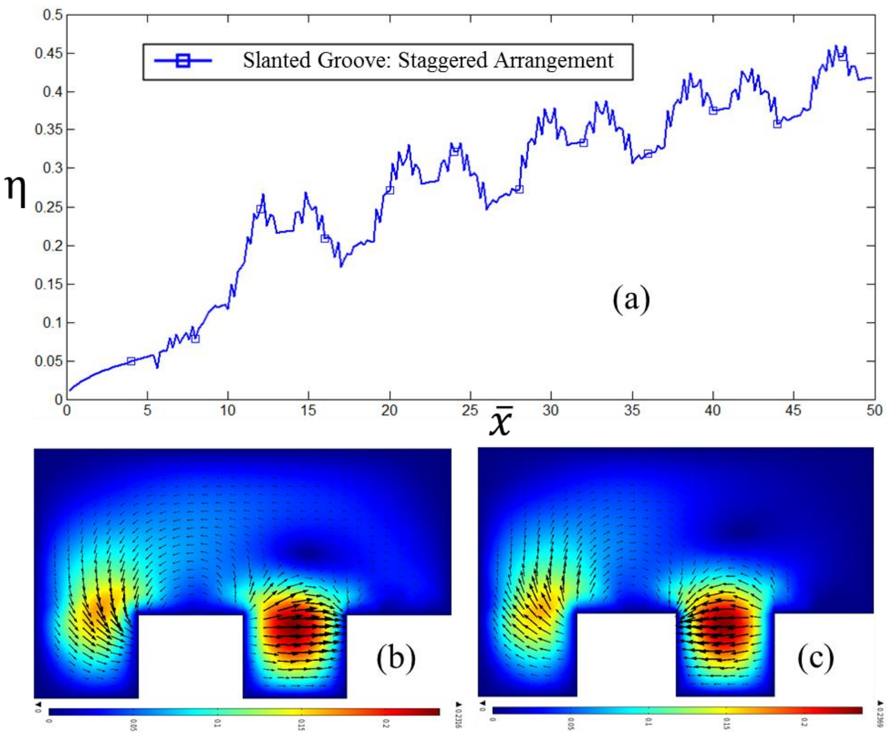


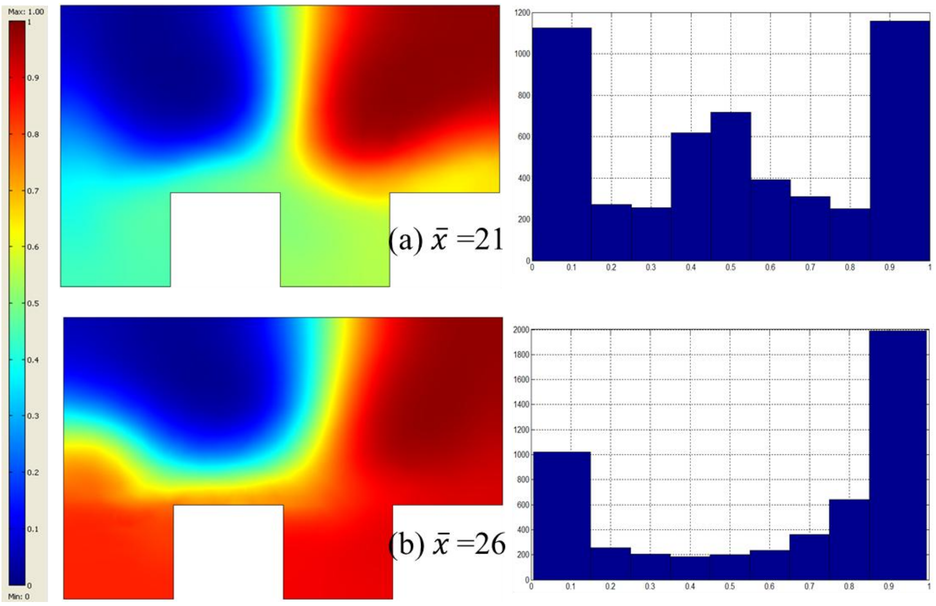




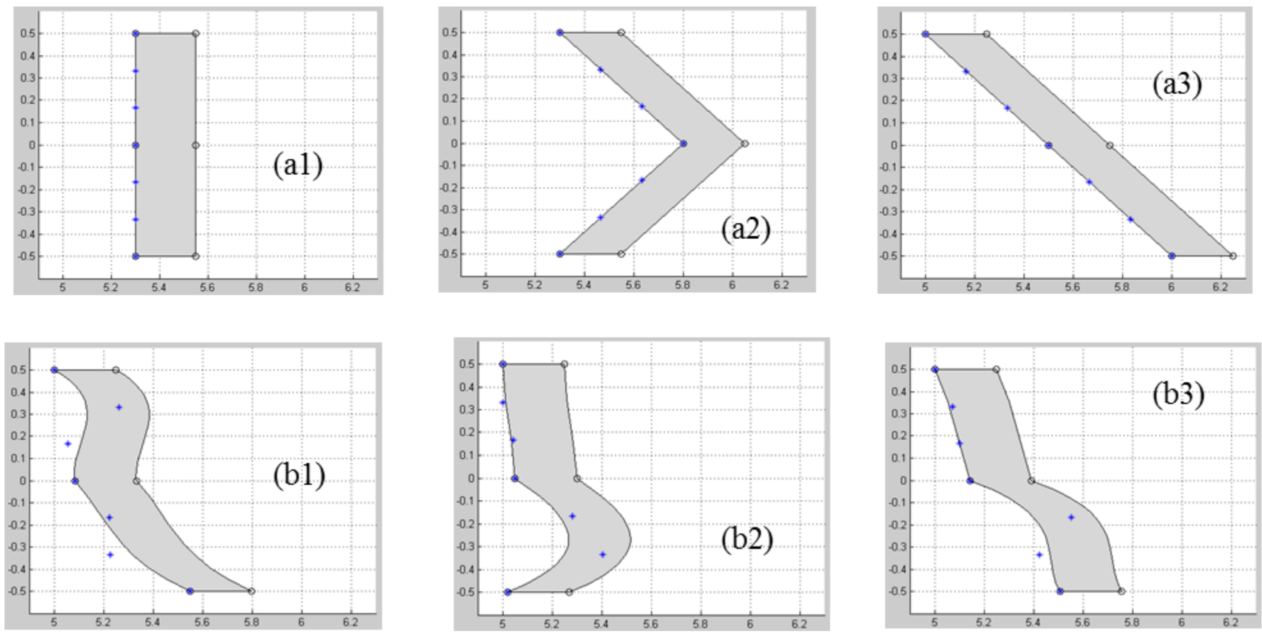
Effect of Flow Reversibility on Mixing Performance







Bézier Curves



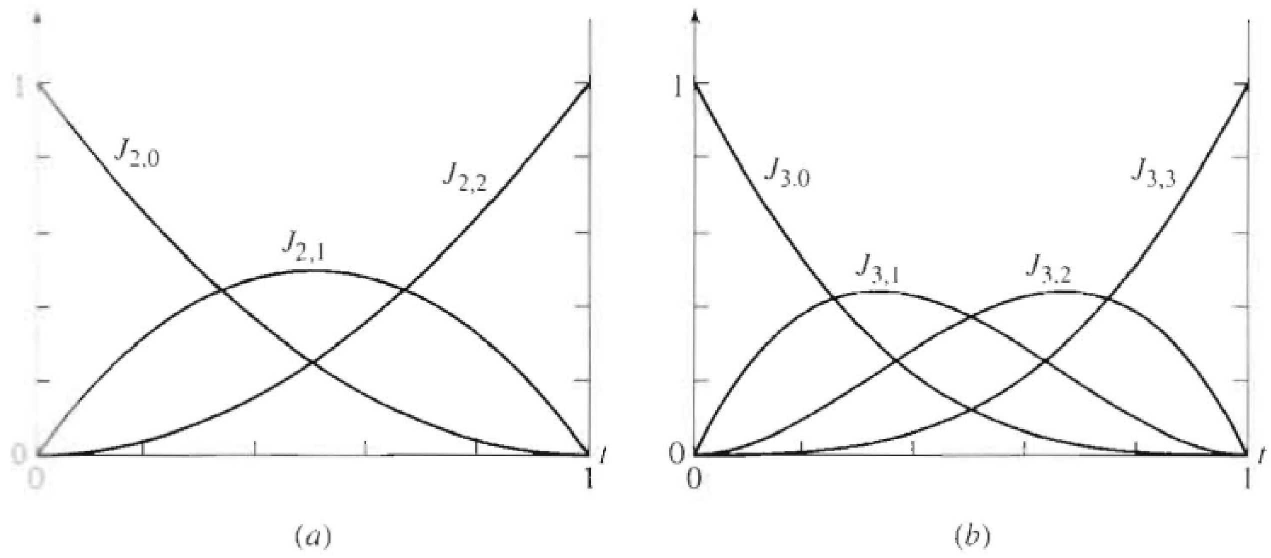
$$P(t) = \sum_{i=0}^{n} B_i J_{n,i}(t) \qquad 0 \leq t \leq 1$$

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

Bézier Curves

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

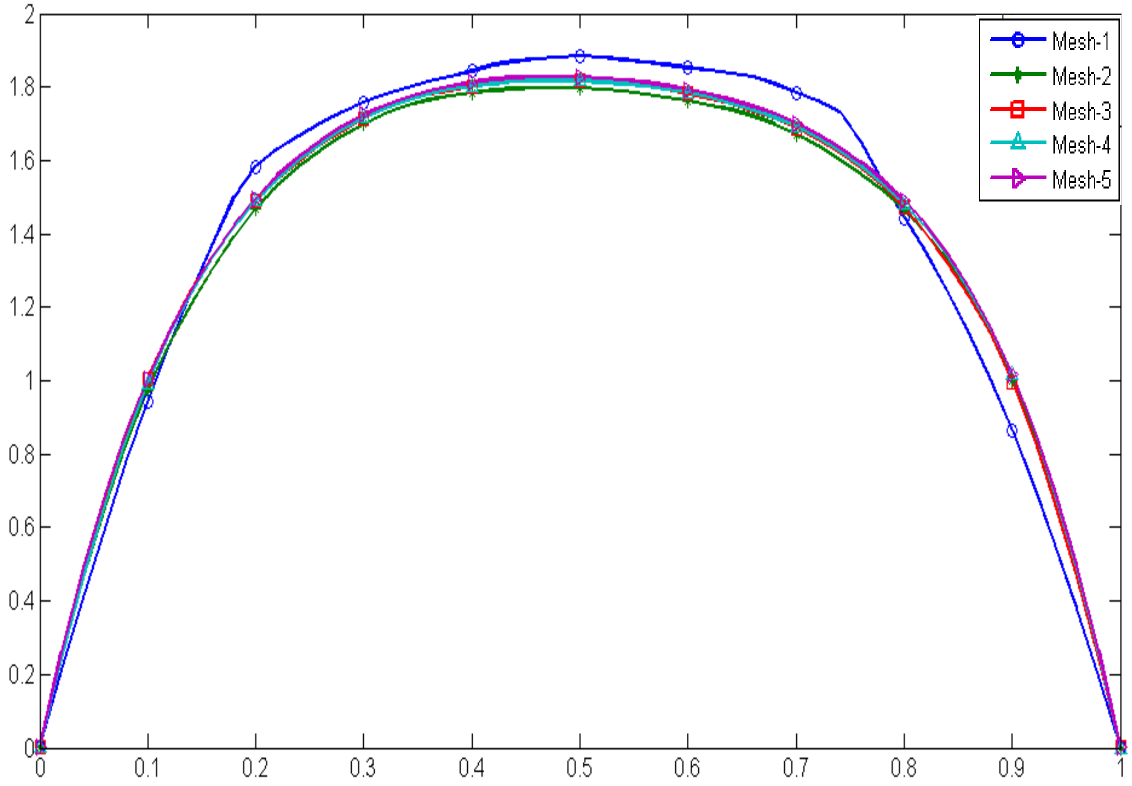
$$J_{n,i}(t) = \frac{n!}{i!\,(n-i)!} t^i (1-t)^{\,n-i}$$



COMSOL CONFERENCE BOSTON 2012

LOUISIANA STATE UNIVERSITY

Mesh Independence and Details



Mesh	No. of Elements	η
1	25k	0.568
2	55k	0.625
3	115k	0.644
4	232k	0.643
5	401k	0.649