COMSOL Conference, Boston, 2013

Brian Vyhnalek, Petru S. Fodor
and
Miron Kaufman

Physics Department
Cleveland State University

Entropic Evaluation of Dean Flow Micromixers

ABSTRACT

We study the use of spiral channels at Reynolds numbers from 25 to 900 as micromixers.

In this system the centrifugal forces experienced by the fluid as it travels along the curved trajectory, induce counter-rotating flows (Dean vortices), needed to promote mixing of chemical species.

The COMSOL Multiphysics and its CFD and Chemical Species Transport modules allows for the simultaneous solving of the Navier – Stokes equations for the fluid flow and the diffusion – convection equations for the concentration of chemical species.

Concentration images obtained at different position along the channel are used to evaluate the mixing efficiency using a measure based on the Shannon information entropy.

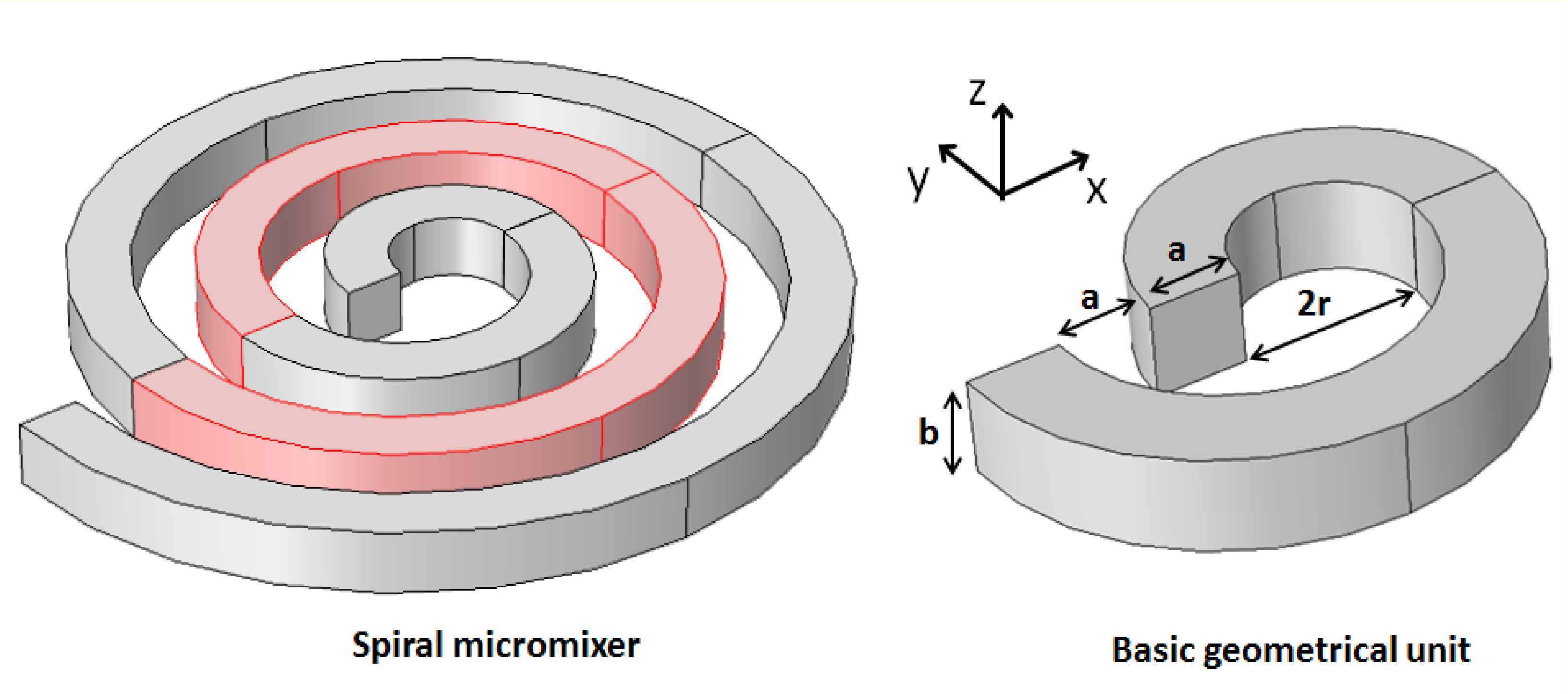
Background

In microfluidic systems the Reynolds number is small, thus the flow is laminar, and promoting mixing is challenging.

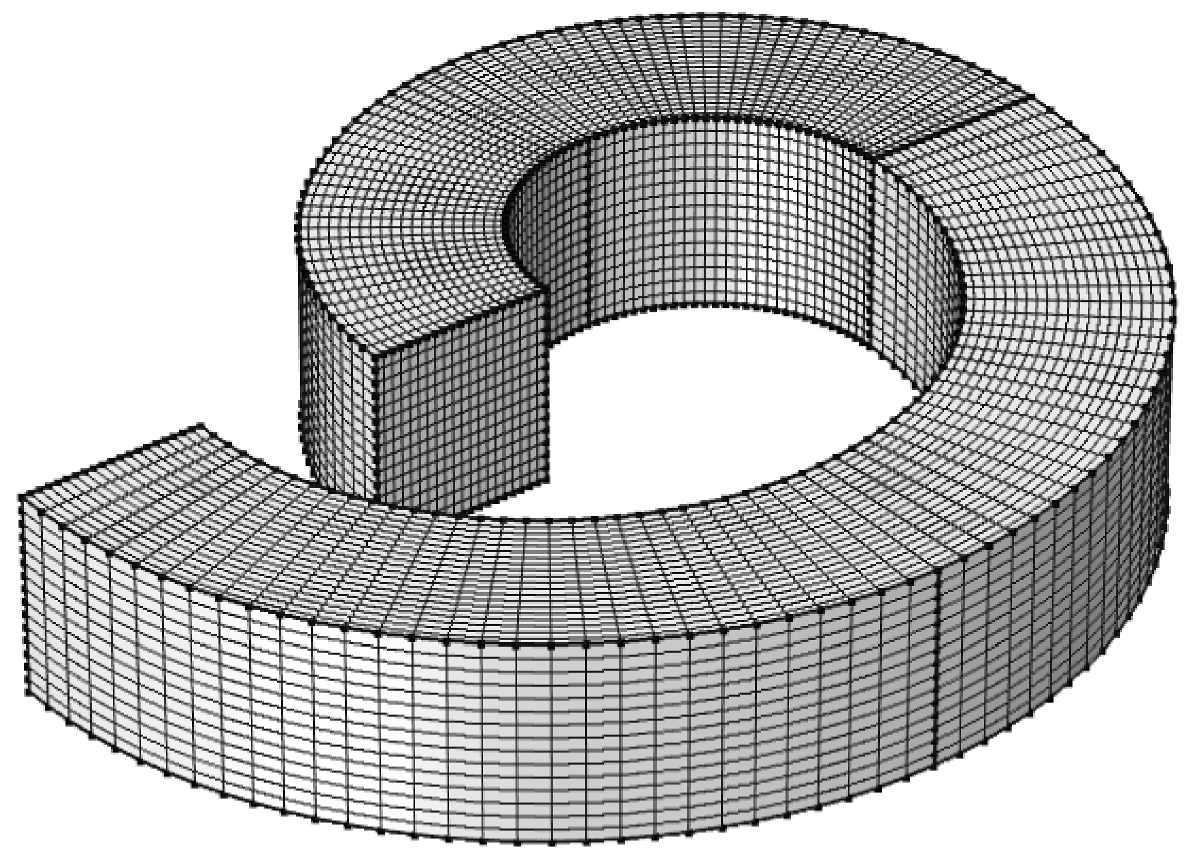
Passive micromixers employ specially designed geometries to increase the contact time and interface area between the various chemical species. They do not involve moving parts and thus have a high degree of reliability and are relatively easy to fabricate. The geometrical structures proposed and used to induce chaotic advection on the microscale are diverse: ridges slanted to the direction of the flow, ridges arranged on a fractal structure, serpentine channels.

Here we analyze the mixing in channels with a spiral geometry. As it moves along the curved channel the fluid experiences centrifugal forces. The superposition of the centrifugal force and the axial pressure gradient creates secondary flows (Dean flows) perpendicular to the primary flow. These secondary flows promote transversal mass transfer within the fluid stream inducing stretching of the interface between the chemical species and at high Reynolds numbers possibly chaotic advection.

Geometrical layout of Dean flow spiral micromixer



Mesh used for the fluid flow modeling



Navier – Stokes equations of motion for an incompressible Newtonian fluid

$$\rho\left[\frac{\partial \mathbf{u}}{\partial t}+(\mathbf{u}\cdot\nabla)\mathbf{u}\right]=-\nabla p+\eta\nabla^2\mathbf{u}$$

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

u = velocity vector
ρ = fluid density
η = fluid viscosity
t = time
p = pressure

The density and viscosity values are set to those for water at room temperature, i.e. 10^3 kg/m3 and 10^{-3} kg/(m s), respectively.

The Convection - Diffusion Equation

The mixing profiles of the two fluids
are visualized using the solution
to the convection – diffusion equation:

$$\frac{\partial c}{\partial t} = D \nabla^2 c - \mathbf{u} \cdot \nabla c$$

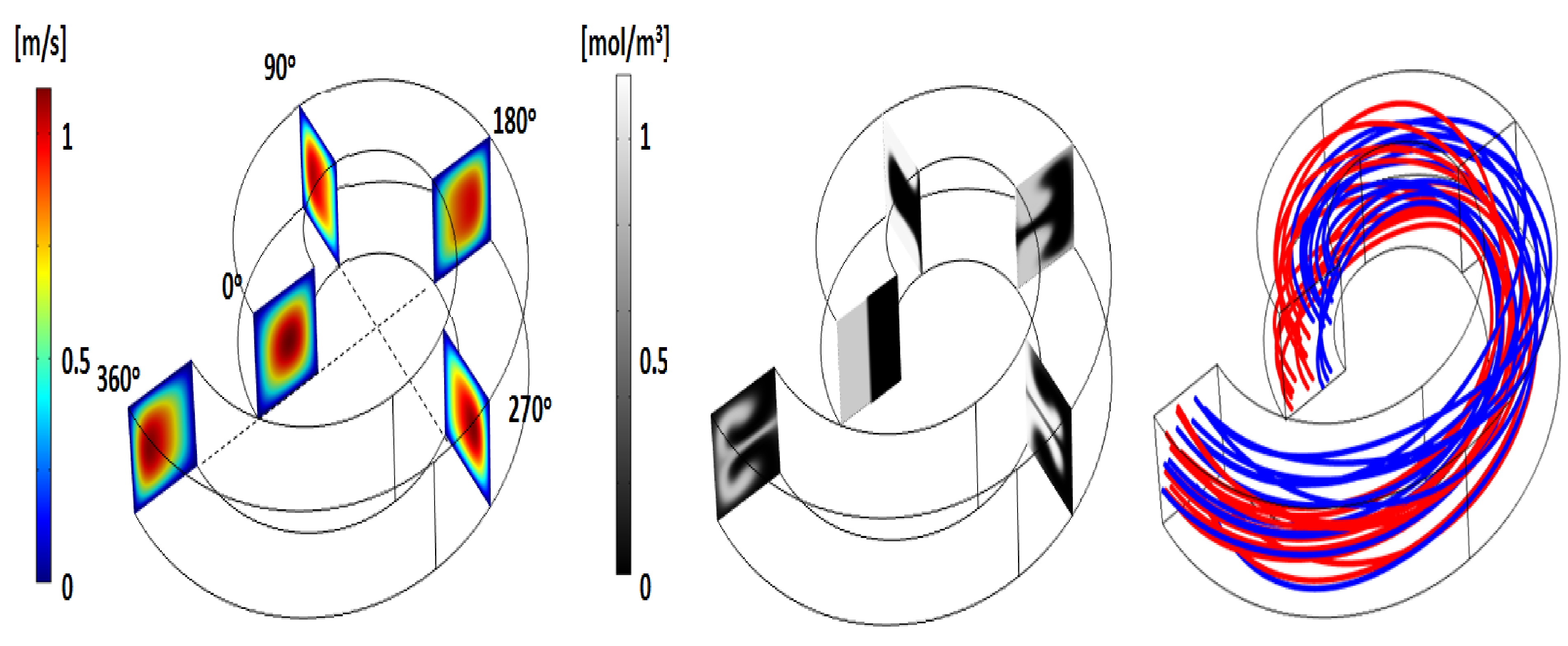
C = concentration of tracers

u = fluid velocity field

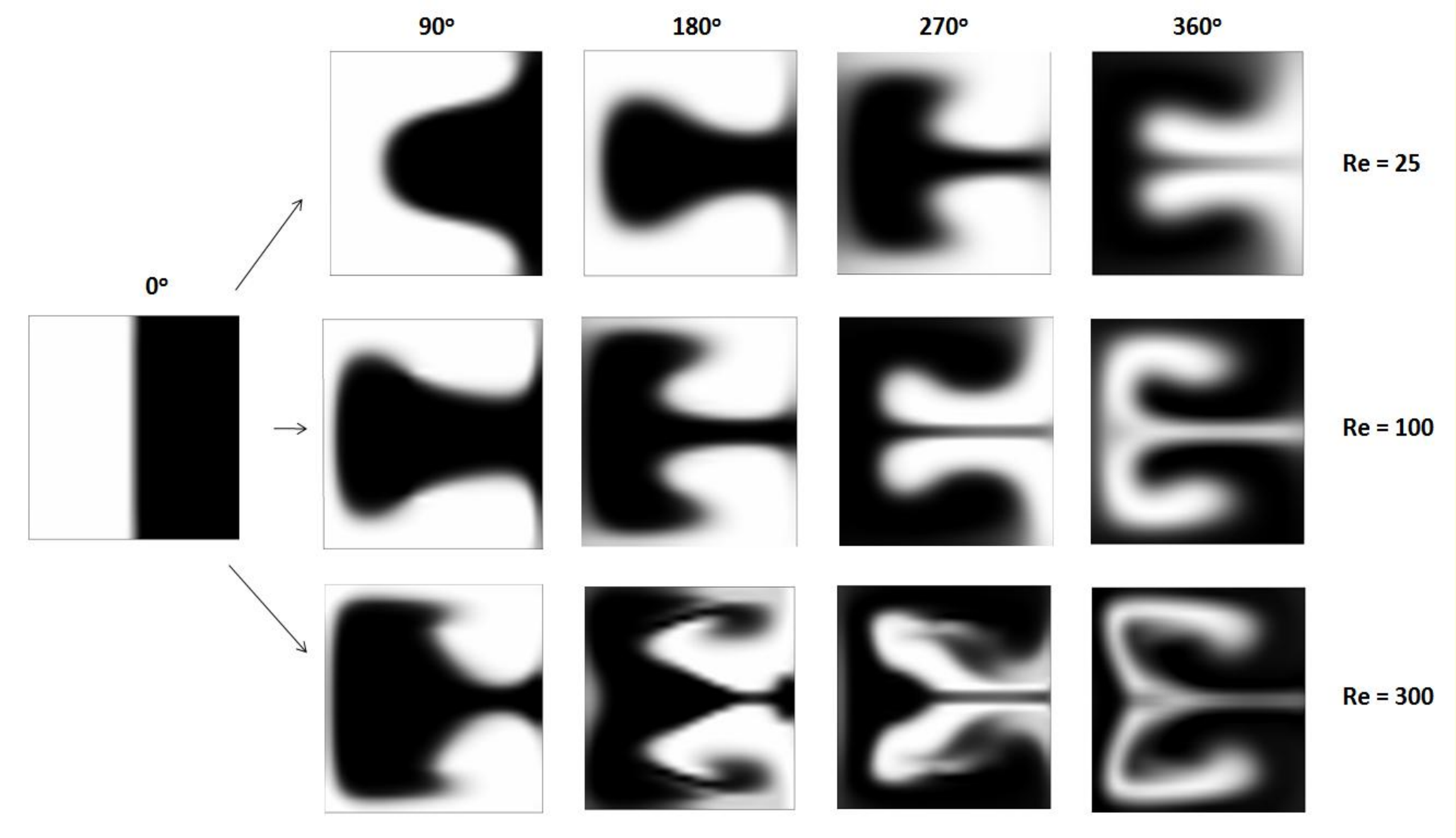
D = diffusion constant.

D = $5*10^{-9} m^2/s$

Simulation Results

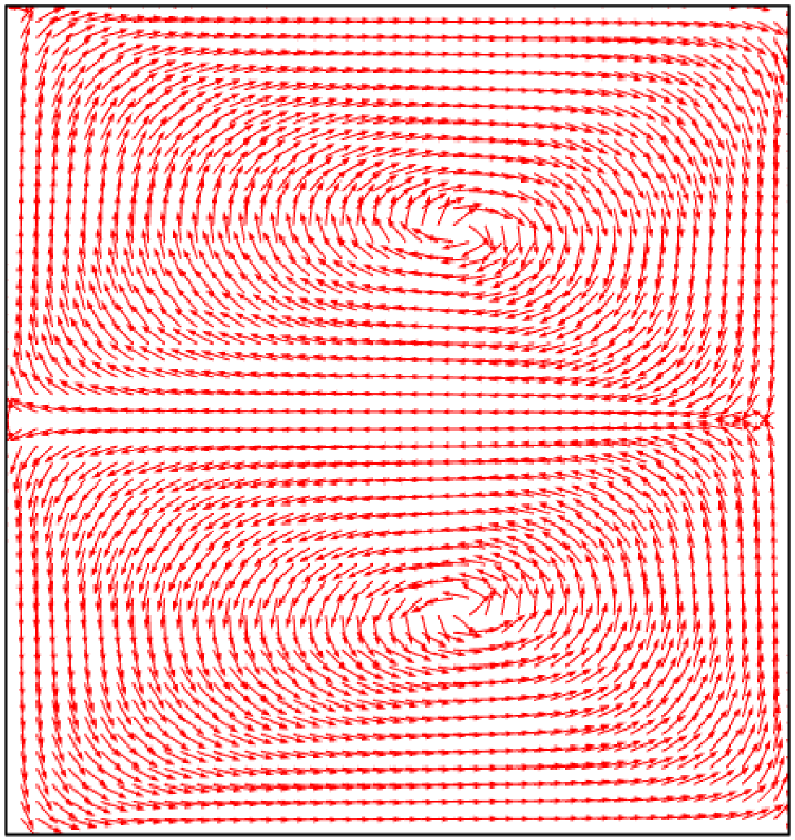


Mixing along the channel

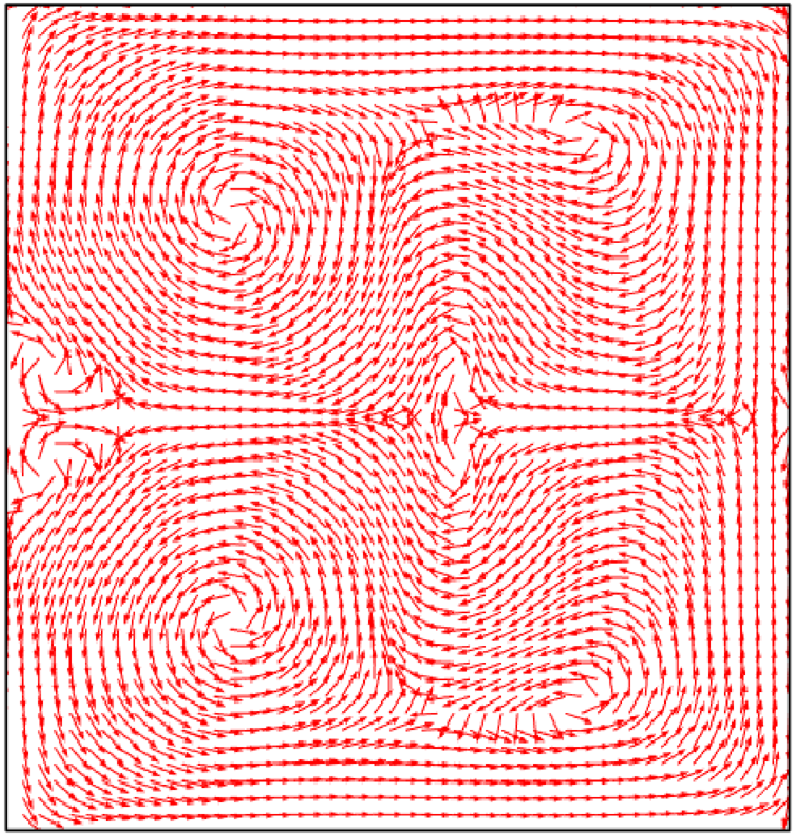


The mixing is promoted by the vortices generated by the centrifugal forces on the fluid.

Flow patterns for different Re

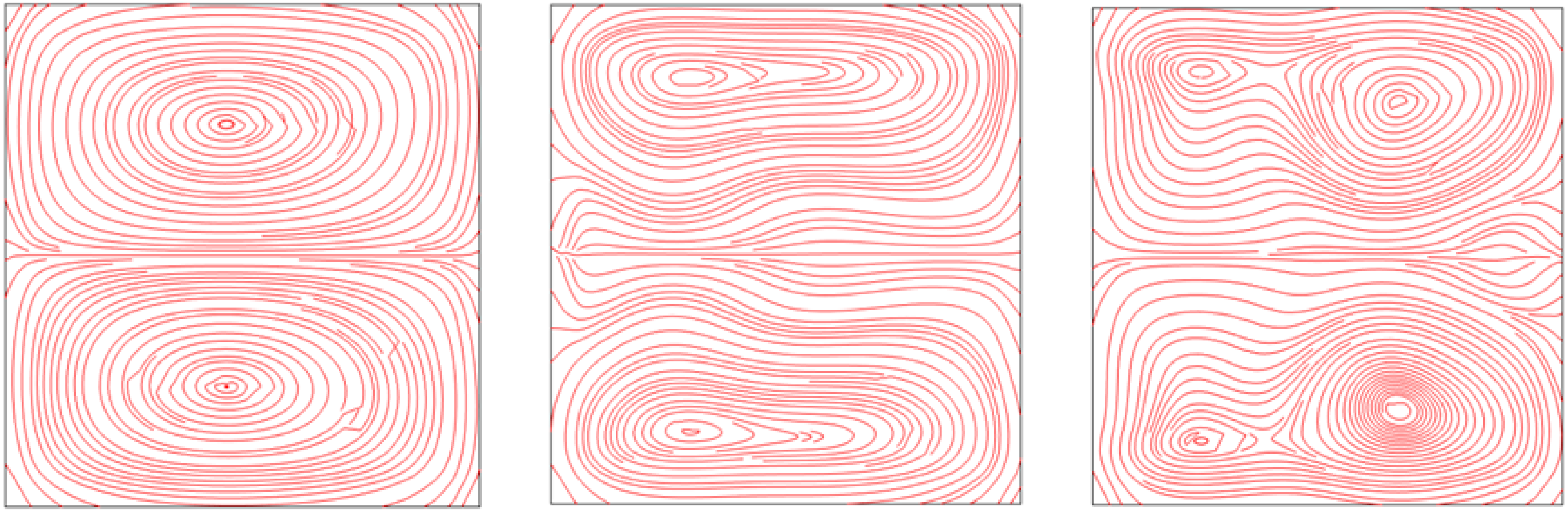


Typical counter-rotating vortex pair, 90^o from the inlet at Re < 100.



As Re is increased above 100, multiple vortex structures appear (Here Re = 500).

Streamline plots at the outlet



Re = 25 Re = 300 Re = 900

Entropic Mixing Evaluation

- To quantify the mixing quality,
  we use an entropic measure
  applied to the concentration images

- The space of interest
  is divided into equal-size regions
  and the fraction of each chemical species
  is evaluated in each regions.

Mixing Entropy and Mixing Index

$$S_{mixing} = -\frac{1}{M}\sum_{j=1}^{M}\left(\sum_{c=1}^{C} p_{c/j}\ln p_{c/j}\right)$$

C = number of chemical species

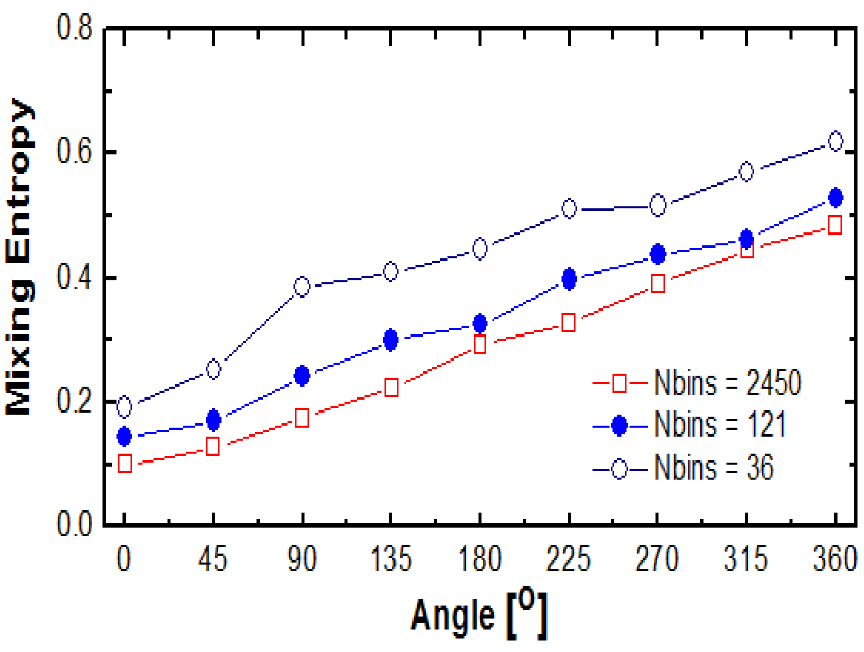
$p_{c/j}$ = conditional probability calculated as the fraction of chemical species of type *c* in bin *j* out of all the chemical species in bin *j*.

Here we have two chemical species C = 2.

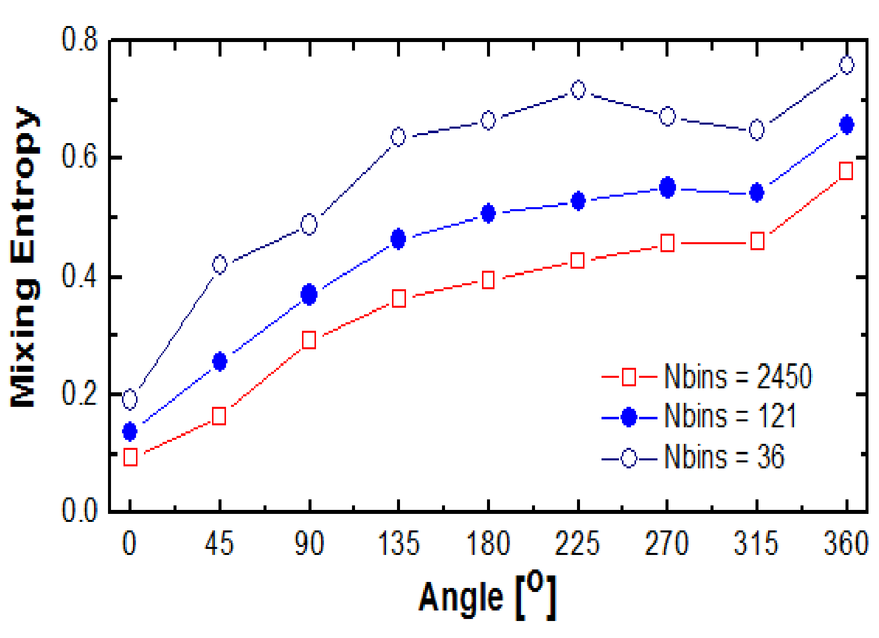
- Its largest value (*S = lnC)* corresponds to the uniform distribution of species through the system and their perfect mixing. By normalizing the mixing entropy S_{mixing} by *lnC*, we define a mixing index varying from 0 (perfect segregation) to 1 (perfect mixing).
- Mixing index = $S_{mixing}/\ln(2)$

Mixing index as a function of the angle

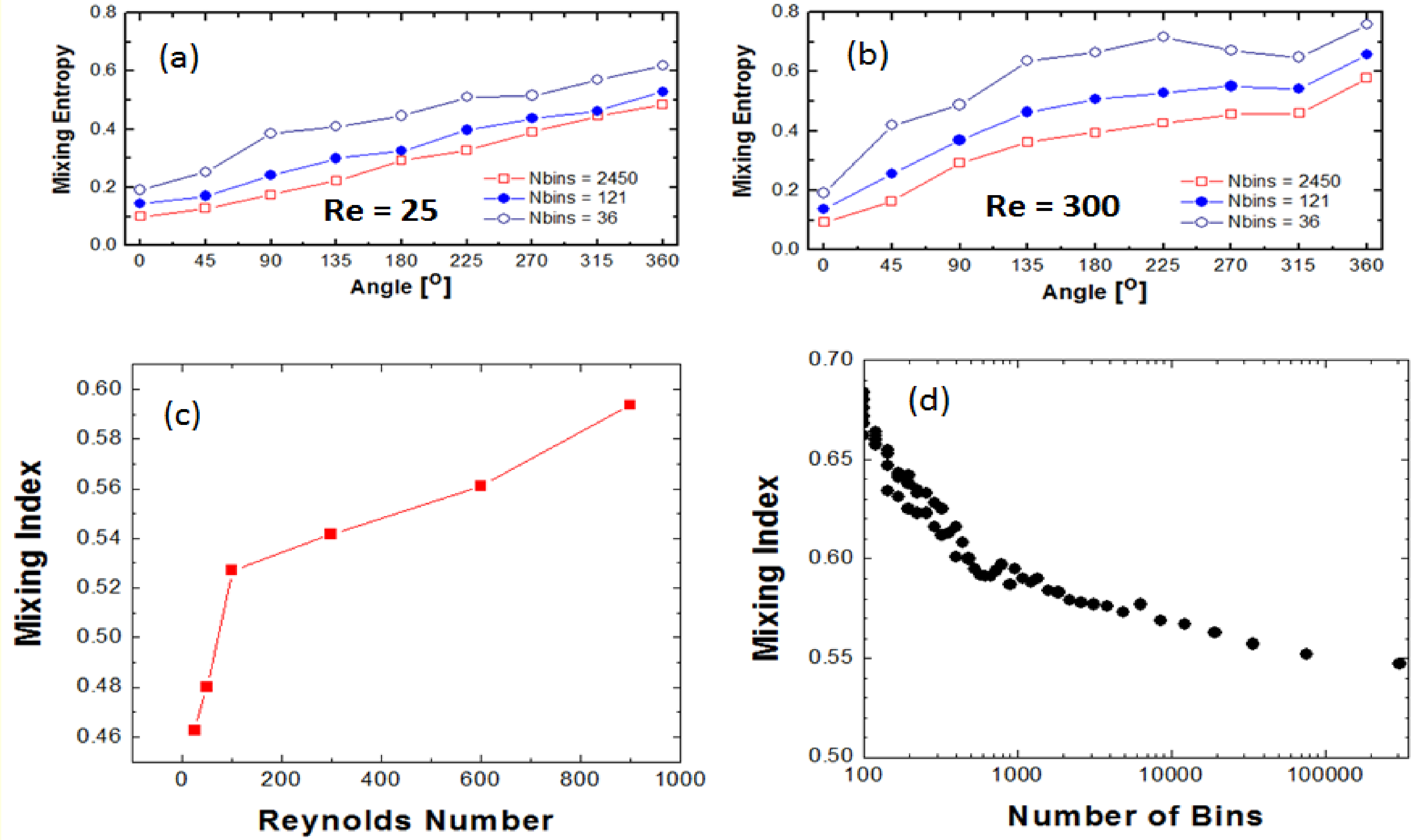
Re = 25



Re = 300



(c)Mixing index vs. Re, at angle of 315^o
(d) Mixing index vs. number of bins (Re = 25, angle = 360^o)



Conclusion

- Modeling of the fluid flow and mass transport using COMSOL + modules has been used to analyze the mixing performance of simple spiral micromixers using an index based on the Shannon information entropy.
- This entropic index indicates that the quality of mixing improves with flow speed, consistent with the emergence of multiple vortex structuress.

References

M. Itomlenskis, P.S. Fodor and M. Kaufman, “Design of Passive Micromixers using COMSOL Multiphysics Software Package”, Proceedings of COMSOL Conference, Boston (2008).

P.S. Fodor, M. Itomlenskis and M. Kaufman, “Assessment of mixing in passive microchannels with fractal surface patterning”, Europ. Phys. J.: Appl. Phys. 47, 31301 (2009).

M. Kaufman and P.S. Fodor, “Fluid mechanics in rectangular cavities – analytical model and numerics”, Physica A 389, 2951 (2010).