

Entropic Evaluation of Dean Flow Micromixers

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Abstract: In the present work, we investigate computationally, using COMSOL Multiphysics and its CFD and Chemical Species Transport modules, the use of spiral channels at Reynolds numbers from 25 to 900, as mixing structures. In this system the centrifugal forces experienced by the fluid as it travels along the curved trajectory, induce counter-rotating flows (Dean vortices). The presence of these transversal flows promotes the mixing of chemical species which are introduced in the system at different positions across the section of the channel. The COMSOL Multiphysics 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 measure¹ based on the Shannon entropy. We have previously found this measure to be useful in understanding mixing in mixers similar with the staggered herringbone type.²

Keywords: Dean flows, micromixers, mixing measures, Shannon entropy.

1. Introduction

Inducing mixing in microfluidic systems is challenging due to their low Reynolds number, and thus laminar nature of the flow. The mixing on these scales relies primarily on the slow diffusion process at the interface between the regions containing the various chemical species. Successful strategies for increasing the mixing efficiency rely both on stretching the mixing interface, as well as promoting advection within the fluid stream.^{3,4} Passive micromixers which employ specially designed geometries to increase the contact time and interface area between the various chemical species, are particularly interesting since they do not involve moving parts and thus have a high degree of reliability and are relatively easy to fabricate. The two basic strategies employed in these mixers are: (i) lamination, i.e. splitting and recombining

components of the fluid stream leading to dynamic maps similar with the baker's chaotic map;⁵ (ii) and promoting chaotic fluid stream motion which is related to the stretching and distortion of the interface between fluid components.⁶

The geometrical structures proposed and used to induce chaotic advection on the microscale are diverse, ranging from groves slanted to the direction of the flow⁷, to zigzag⁸ and serpentine channels.⁹ In this particular work we analyze the mixing in channels with a spiral geometry (Figure 1). Writing the momentum equations for this type of geometry indicates that as it moves along the curved channel the fluid experiences centrifugal body forces:

$$\vec{F}_c = \frac{\rho v^2}{r} \cos \theta \cdot \hat{r} - \frac{\rho v^2}{r} \sin \theta \cdot \hat{\theta} \quad [1]$$

in the radial and theta directions. The superposition of the centrifugal force and the axial pressure gradient creates secondary flows (Dean flows)³ 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.

2. Solving the Governing Equations in COMSOL Multiphysics

The transport of chemical species through the basic unit (a full 360 degrees turn) of the spiral microchannel is analyzed by solving the Navier – Stokes and the convection-diffusion equations:

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

$$\nabla \cdot \mathbf{u} = 0 \quad [3]$$

$$\frac{\partial c}{\partial t} = D \nabla^2 c - \mathbf{u} \cdot \nabla c \quad [4]$$

where \mathbf{u} - velocity vector, ρ - fluid density, η - viscosity, t - time, p - pressure, c - concentration

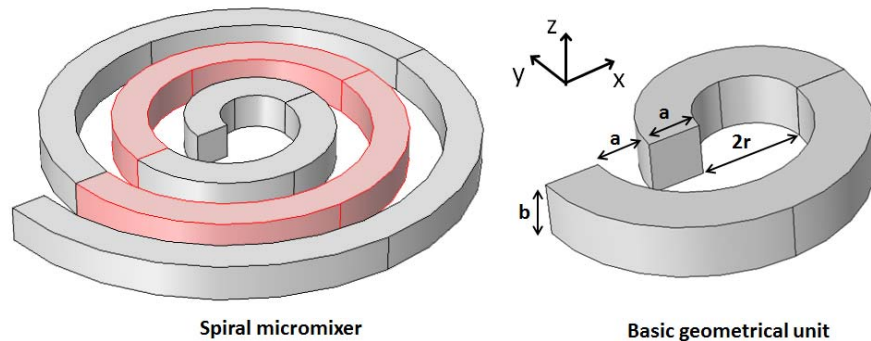


Figure 1. Geometrical layout of Dean flow spiral micromixer investigated.

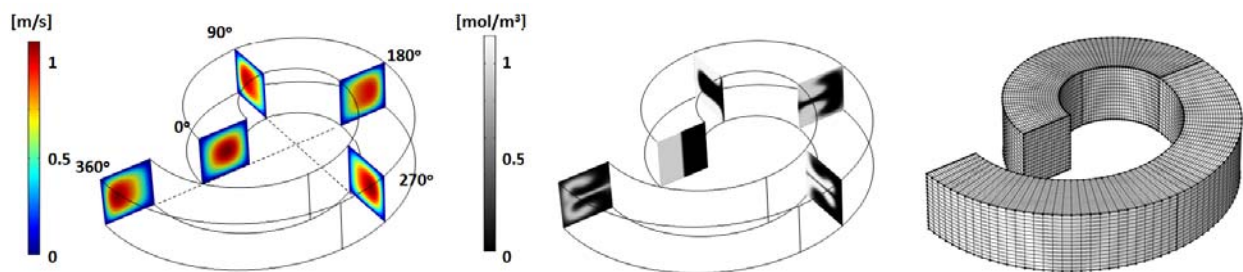


Figure 2. (left) Velocity field; and (middle) concentration slices for a microchannel at Reynolds number $Re = 50$ ($a = b = 100 \mu\text{m}$; $r = 100 \mu\text{m}$) (Note: the 0° angle corresponds to the inlet of the mixer). (right) Mapped meshing used in the fluid flow simulations.

and D is the diffusion constant ($= 5 \times 10^{-9} \text{ m}^2/\text{s}$ for all the simulations). The flow and convection-diffusion equations are solved using the COMSOL Fluid Dynamics module and the Chemical Species Transport module, respectively. Both physics are solved using a generalized minimal residual method (GMRES) iterative solver with a geometrical multigrid preconditioner and a Vanka algorithm for the pre- and post-smoothing. The typical number of elements in the mesh used for the flow field is 60,000, which in the limit of low Reynolds numbers ensures that the element size is sufficiently small for the solution to be independent on the mesh size. For the convection-diffusion equation the mesh used is much denser ($\sim 224,000$), to avoid the possible numerical errors that can be associated with this type of problem. For both meshes we have used mapped meshes on the inlet and top side of the channel and then swept them through the entire geometry (Figure 2). This allows a high resolution for the discretization of the cross

section of the channel, while limiting the total number of elements needed for the model.

3. Methods – Mixing Analysis

Quantizing mixing has been a central research problem for many years, given its direct relevance for processes ranging from chemical reaction engineering, to polymer processing and blending of multiphase systems. While a consensus on a single mixing measure is still to be reached,^{10,11} some of the qualities that such a method of quantification should have include: rigorous mathematical underpinning, applicability to any physical process involving mixing, and flexibility to the various formats in which data about the distributions of the components in a multiphase system is extracted. On the later point, in many simulations involving multiple chemical species, their distribution is encoded either in intensity maps generated based on the reactants' concentration, or in the position of tracers released at different positions within the system and carried by the flow. If the quality

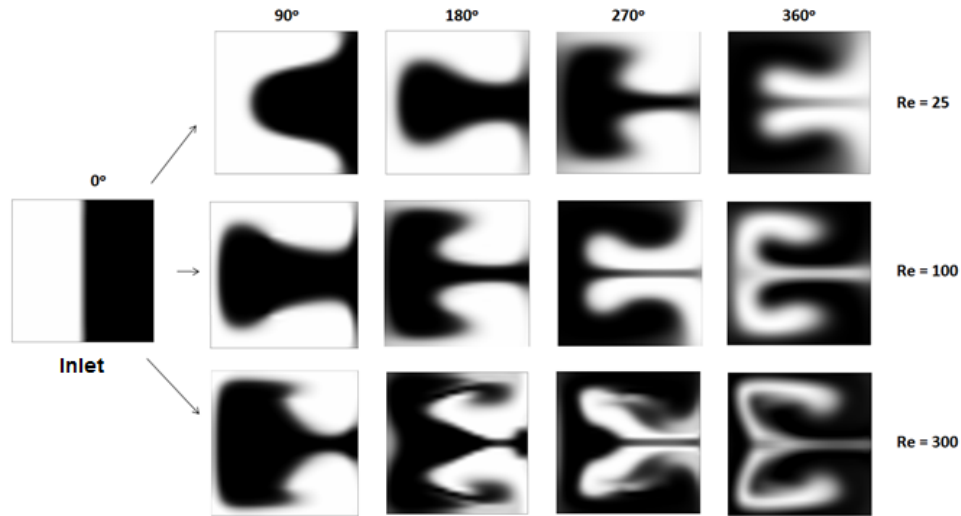


Figure 3. Snapshots of the mixing along the channel of two fluids introduced at different positions across the inlet of the curved geometry.

of mixing is to be analyzed in a consistent manner, the mixing measure used should be easily adapted to concentration maps obtained by solving the convection-diffusion equation, or the Poincaré maps obtained by solving the equation of motion for tracers. The particular method used to measure mixing in this work, is based on calculating the Shannon informational entropy associated with the distribution of various species across the cross-section of the channel. To calculate this measure the concentration images at different position along the channel are divided into a number N_{bins} of equal size regions and the fraction of each of the chemical species is evaluated in each of these regions. The mixing entropy is then calculated as^{12, 13}:

$$S_{mixing} = -\frac{1}{M} \sum_{j=1}^M \left(\sum_{c=1}^C p_{c/j} \ln p_{c/j} \right) \quad [5]$$

where C is the number of chemical species and $p_{c/j}$ is a conditional probability calculated as the fraction of chemical species of type c in bin j out of all the chemical species in bin j . In this particular study we have two chemical species $C = 2$, and the conditional probabilities are normalized: $p_{2/j} = 1 - p_{1/j}$. The lowest value ($S_{mixing} = 0$) corresponds to each bin containing at most one type of chemical species, i.e. perfect segregation between the components. Its largest value ($S = \ln C$) corresponds to the situation in which bins contain equal concentrations of the chemical species, i.e. $p_{c/j}$ are all equal to each

other in these bins^{2,12-14}. Physically this corresponds to the uniform distribution of species through the system and their perfect mixing. By normalizing the mixing entropy S_{mixing} by $\ln C$ (i.e. $\ln 2$ in this particular case, since we use two chemical species), the mixing index will take values from 0 to 1, with 0 corresponding to a completely segregated system, and 1 corresponding to perfect mixing, respectively.

4. Discussion

Figure 3, shows snapshots of the concentration of one of the chemical species at different positions along the channel for different Reynolds numbers. The positions are identified by the polar angle of the corresponding cross section, with the 0 degree position corresponding to the inlet. In all cases the reactant species are introduced on separate sides of the inlet. Even at low Reynolds numbers, it is immediately apparent that as the fluid moves along the curved channel, the presence of the centrifugal forces leads to a stretching of the interface between the chemical components. As shown in Figure 4, this is due to the formation of counter-rotating flows on the top and bottom sides of the channel. It has to be noted that at Reynolds numbers $Re < 300$, the interface remains continuous with a length proportional with the position along the channel

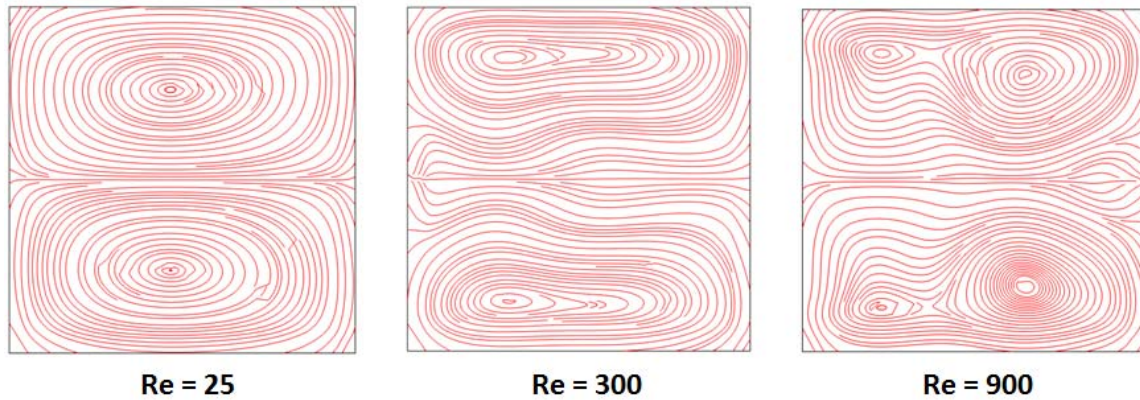


Figure 4. Streamline plots based on the transversal components of the fluid velocity at the outlet of the Dean flow micromixer.

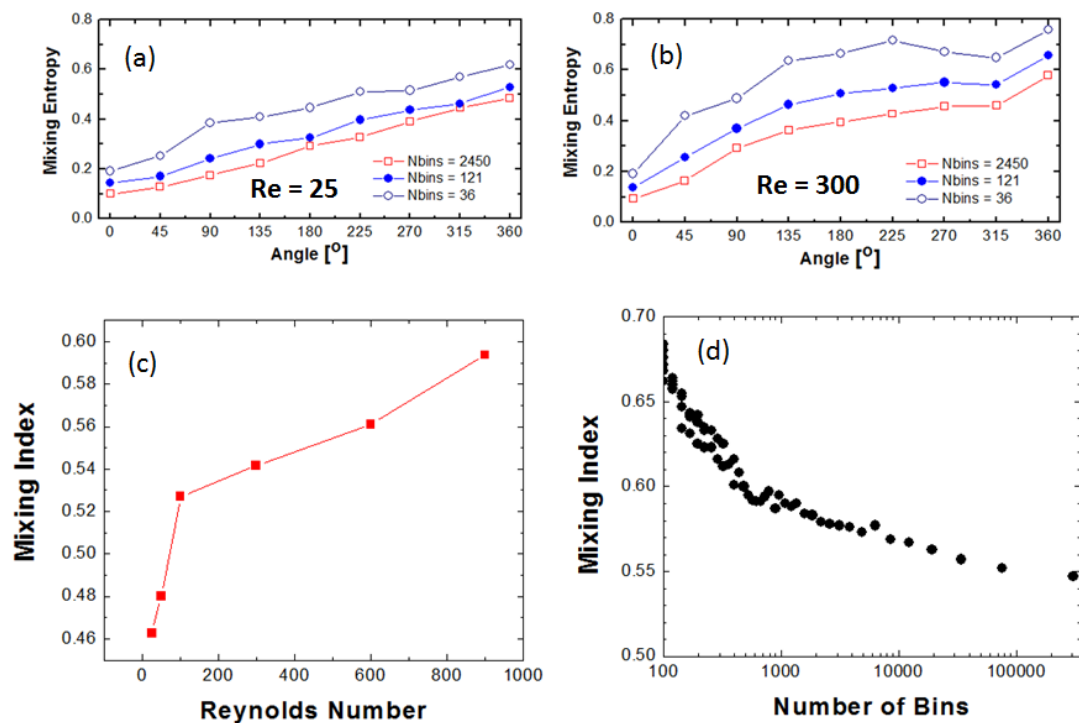


Figure 5. Mixing index as a function of the angle at (a) $Re = 25$ and (b) $Re = 300$; (c) Dependence of the mixing index on the Reynolds number, as measured from cross sections at angle 315° (data shown is for $N_{bins} = 121$); (d) Mixing index dependence on the number of bins used ($Re = 25$, angle = 360°)

and the magnitude of Re , i.e. the strength of the centrifugal forces. However as the Reynolds number is increased the flow structure changes as indicated by the breakup of the interface and the development of striations in the concentration profiles. An analysis of the cross-sectional streamlines (Figure 4), shows that the changes in the flow structure occurring at Reynolds numbers exceeding $Re = 300$,

correspond to the formation of multiple vortex pairs and crossover points indicative of chaotic advection.

Calculation of the entropy based mixing index (Figure 5), shows that the quality of mixing is improved as the Reynolds number is increased consistent with the combined effect of the increase spatial contact between the different chemical species and the formation of striations

in their distribution (Figure 5). Besides the dependence on the Reynolds number, the entropy based mixing index also depends on the bin size. This dependence on the scale of observation is expected given the decrease in the probability of finding different components in the same region as the bin size decreases.

5. Conclusion

Modeling of the fluid flow and mass transport using the COMSOL Multiphysics package¹⁴ and its associated modules has been used to analyze the mixing performance of simple spiral micromixers using a rigorously defined mixing index based on the Shannon information entropy. This entropic index indicates that the quality of mixing is improved as the flow speed is increased, consistent with the development of multiple vortex structures within the fluid stream. Future work will focus on using this entropy based index as a tool to compare the performance of various mixer designs, and on the understanding of its dependence on the scale of observation.

6. References

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