Design of Passive Micromixers using the COMSOL Multiphysics software package

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Abstract: Relief patterning of the surface of microchannels has been actively pursued as a method of promoting mixing in systems with a low Reynold's number (<<100). For example, structures such as the staggered herring bone (SHB), which consists of periodic groves and ridges distributed along the channel length, improve mixing by inducing counter – rotating helical flows in pressure driven systems.

In this work, we explore by using the COMSOL Multiphysics package and its Chemical Engineering Module, the possibility of enhancing the mixing quality of two fluids in a microchannel with a non-periodic fractal pattern of ridges on the channel bottom. The quality of the mixing between two fluids is quantified with an entropic measure. For the binary fluid system, we compare the mixing performance of channels with ridges locations determined by employing a Weierstrass fractal function, to the performance of SHB designs. The mixing efficiency associated with the Weierstrass function based designs is consistently better than for the SHB counterparts.

Keywords: microfluidics, staggered herring bone mixer, fractals, entropy.

1. Introduction

The design and fabrication of microfluidic analytical devices has potential applications for chemical synthesis and analysis, DNA or protein analysis and drug discovery.[1,2]

One of the basic requirements for microfluidic systems is the capability of efficiently mixing different fluid components. Since the values for the Reynolds number in microchannels is small and thus the fluid flow in a pressure driven system is laminar, one needs to design geometries for the channels that will induce transversal flows and mixing.

Stroock et al[3] have demonstrated that asymmetric V-shaped groves patterned on the bottom of a straight rectangular channel present an anisotropic resistance profile to the fluid flow allowing the pressure differential between the inlet and outlet of the channel to induce transversal components within the flow. These transversal components of the flow field promote mixing of different fluid components within length scales of the order of centimeters making the designs compatible with lab-on-a-chip applications.

In the current study we follow up on the idea of Camesasca et al[4] to enhance mixing by replacing the periodic structure of ridges with a non-periodic one, as described below.

2. Microchannel geometry

In this study we have investigated mixing in rectangular channels 5000 μm in length, 200 μm in width, and 150 μm in height (Figure 1). The height of the asymmetric V-shaped ridges placed on the bottom of the channels is fixed at 50 μm. While the ridges are distributed uniformly along the direction of the flow through the channels, their y – position is non - periodic and is generated using the Weierstrass function defined as follows:

$$W(x) = \sum_{n=0}^{\infty} \frac{\sin(2^n x)}{2^{n(2-D)}} \qquad [1]$$

This function is evaluated in MathCad for different fractal dimensions D and then sampled for the desired number of points (Figure 2). The ridge design is completed by constraining their geometrical arms to make 45^o angles with the channel's long axis.

For the purpose of comparison, for each of the fractal based design studied, a SHB design with the same geometrical parameters, i.e. ridge spacing and apex range, was also investigated.

3. Flow field modeling

The flow fields for each structure were modeled using the COMSOL Multiphysics package and its Chemical Engineering Module.

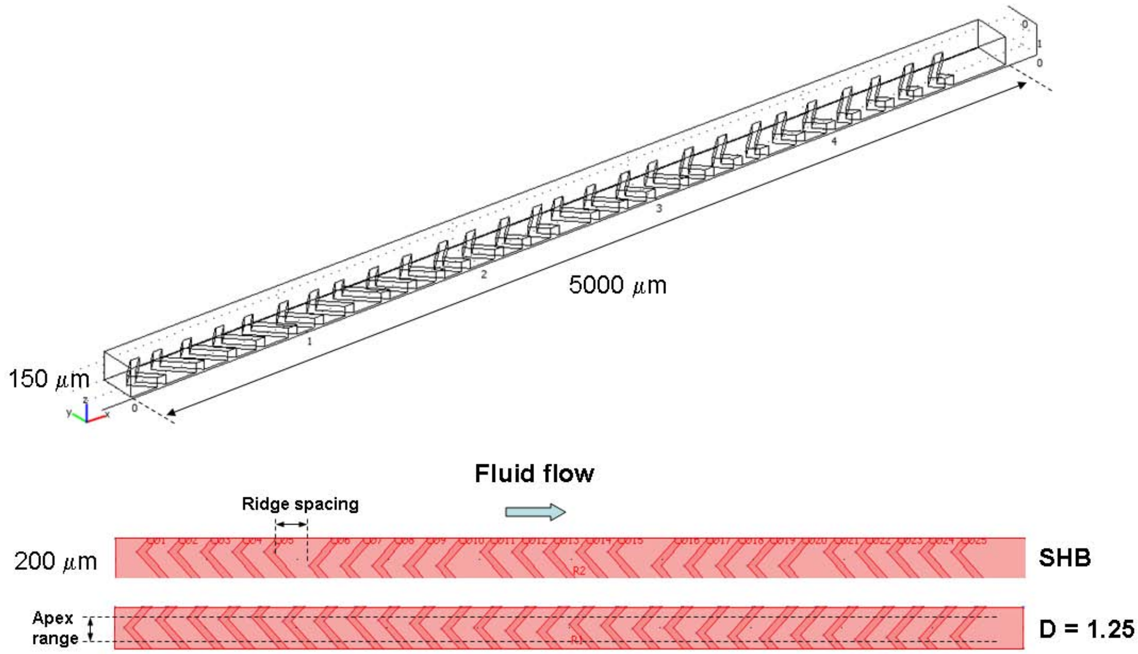

Figure 1. (Top) 3D geometry for rectangular microchannels. (Bottom) Comparison between the ridge profiles for the staggered herring bone (SHB) and fractal designs (Ex. D = 1.25).

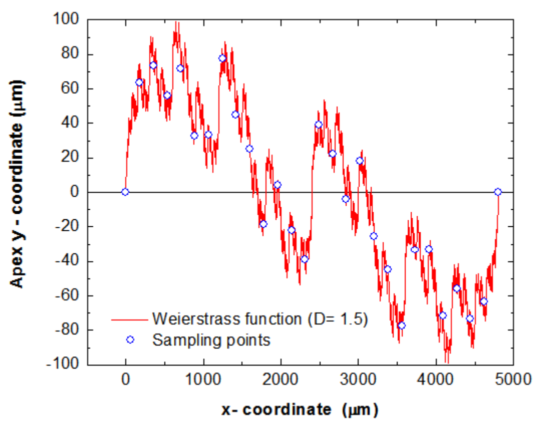

Figure 2. Coordinates for the y – position of the ridge apex calculated using a Weierstrass function of the form described in the text (D = 1.50, ridge spacing = 150 µm).

The flow fields are obtained solving the Navier – Stokes equations of motion for an incompressible Newtonian fluid:

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

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

where **u** is the velocity vector, ρ is the fluid density (10^3 kg/m^3 for water), η is the fluid viscosity (10^{-3} kg/(m s) for water), *t* is the time, and *p* is the pressure. The equations are solved for a steady state flow with the following boundary conditions: (1) 0.01 m/s inlet velocity oriented along the long axis of the channel; (2) no slip at all the solid surfaces; and (3) zero pressure at the outlet. The equations are solved using the GMRES solver for a mesh with a typical number of elements of 60,000.

Figure 3 shows cross – sections of the velocity field along the channel length. As expected, for a rectangular channel without surface patterning the velocity field profile is symmetric and parabolic with only longitudinal components (along the flow direction) for the velocity. On the other hand for all the designs with bottom surface patterns, the resistance to the flow imposed by the V-shape ridges, disturbs the global axial movement of the fluid and induces transversal components within the velocity field. The counter-rotating transversal flows thus created, can dramatically enhance the contribution to the mixing of fluids due to convection.

4. Fluid mixing

The mixing profiles of two fluids are visualized by solving the convection – diffusion equation and particle tracing.

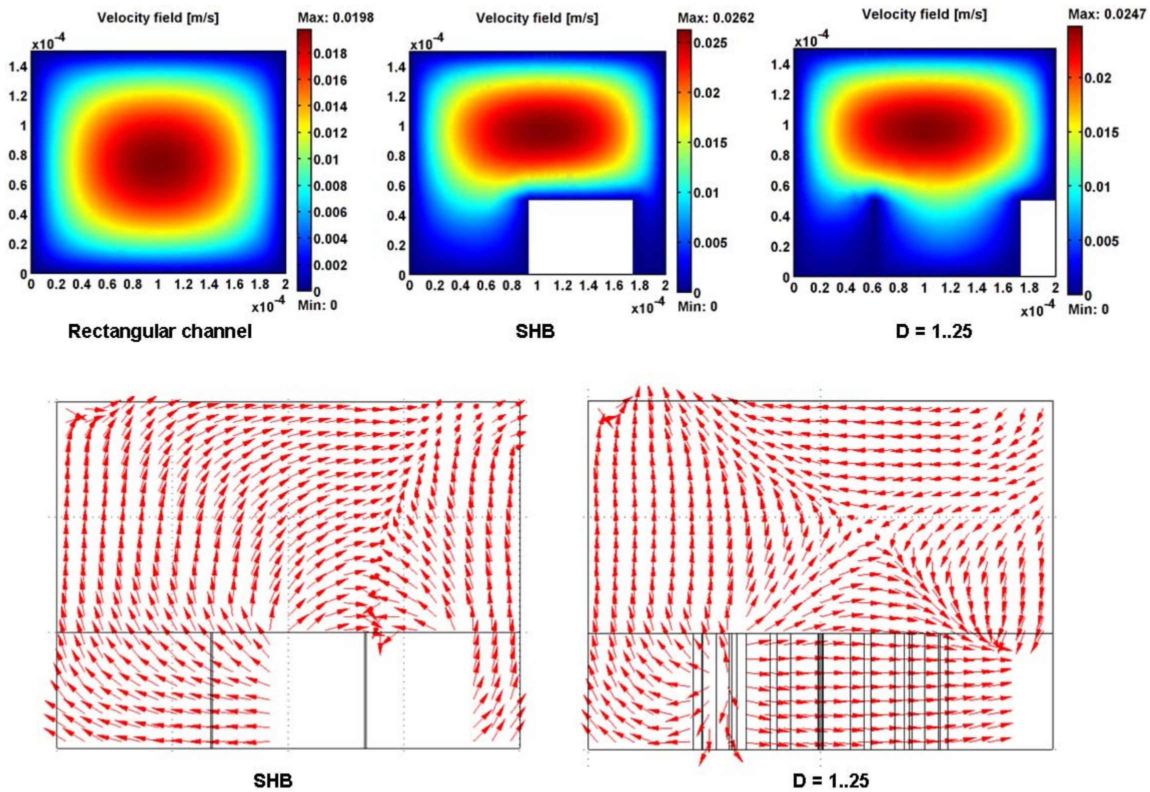

Figure 3. (Top) Velocity field cross – sections at x = 1450 μm for a rectangular channel with and without bottom ridges. (Bottom) Transversal components of the flow for the staggered herring bone (SHB) and D = 1.25 design (x – coordinate = 1450 μm)

In the first approach the convection – diffusion equation is solved in the steady flow state with a discontinuous concentration profile across the inlet generated using a Heaviside step function:

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

where c is the concentration, D is the diffusion constant, and **u** is the vector field. The solution for the velocity field is determined independently by solving the Navier – Stokes equations for the given geometry. Subsequently, the solution stored is used to solve the convection-diffusion equation for the steady state. The mesh used in this case is denser (~140,000 elements) in order to account for the high concentration gradients at the interfaces between the two fluids. The equation is solved using the direct solver based on Gaussian elimination, for diffusion constants fixed in the range 0.5 – 1.2 x 10^{-9} m^2/s. Using smaller values, than the above mentioned ones, for the diffusion constant typically leads to large numerical errors in the solution.

As shown in Figure 4 for the rectangular channel without ridges the mixing is purely diffusive with no contribution from convection. In the absence of transversal components in the flow fields the mixing is limited to the initial interface between the two fluids. Nevertheless, in designs employing surface patterns, the mixing is greatly enhanced and is driven by the convective effects associated with the transversal flows generated by the asymmetric ridges. While mixing through diffusion still occurs at the interface between the two fluids its contribution to the total mixing represents only about 10 % of the total mixing. This conclusion is also supported by visualizing the mixing using particle tracing. The trajectories of massless particles (~8000) released with a uniform density across the inlet of the channel, are obtained using the particle tracing feature of the COMSOL package.

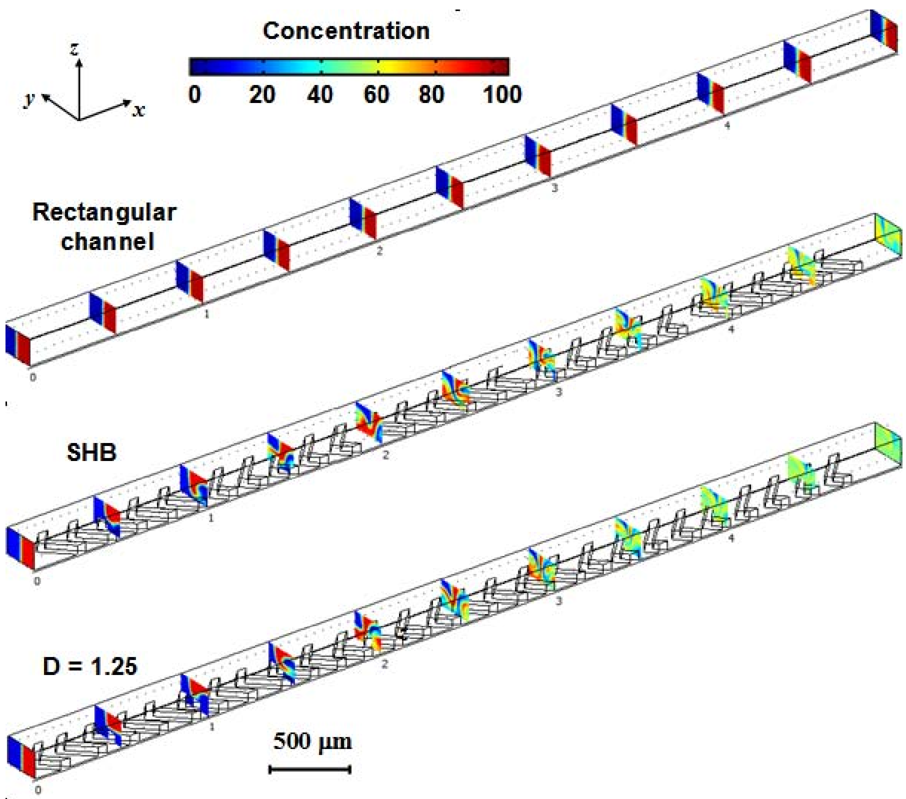

Figure 4. Concentration profiles at different positions along the length of the channel for a design without ridges, for a SHB design and for a fractal pattern design with D = 1.25

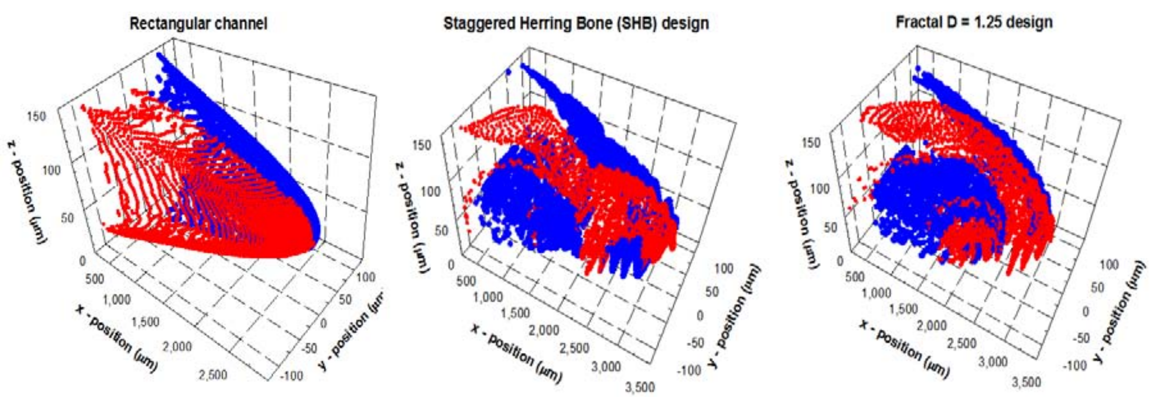

Figure 5. Positions of two sets of tracers at t = 0.15 s. The two sets of tracers are released on separate sides of the inlet.

As seen in Figure 5, a snapshot of the particles' positions after a set time from release shows only little crossover between the sets of particles released on the two sides of the inlet In essence in the yz - plane the interface between the two sets of particles remains unchanged as they propagate along the channel. On the other hand, in channels in which the geometrical features disturb the laminar flow of the fluid, the particles trajectories deviate strongly from straight lines leading to the intermixing between the two sets of particles.

5. Mixing evaluation

While concentration or tracer images clearly indicate the capability of all the designs with patterned ridges, that have been investigated, to enhance the mixing of two fluids, in order to rate their relative performance, we are using an entropic measure that quantifies the mixing quality.

Following Camesasca et al[5], we are using the entropy to quantify mixing:

$$S_{locations}(species) = \sum_{j=1}^{M} p_j S_j(species) \qquad [5]$$

with:

$$S_j(species) = -\sum_{c=1}^{2} p_{c/j} \ln p_{c/j} \qquad [6]$$

$p_{c/j}$ is the probability of finding a tracer of species c conditional on being in region j and p_j is the probability of a tracer, irrespective of species, to be in bin j. $S_j(species)$ is the entropy of mixing the two species of tracers at the location j and $S_{locations}(species)$ is a spatial average of the entropy of mixing of tracers species conditional on location. Since $0 \le S_{locations}(species) \le \ln(2)$, we get a mixing index, $S_{locations}(species)/\ln(2)$, which takes values between 0 (perfect segregation) and 1 (perfect mixing).

The entropy expressions are evaluated in Mathcad using the concentration profiles exported from COMSOL. Each concentration cross – sectional profile is computed using M = 30,351 bins, which is sufficiently large to ensure that the mixing index is independent of the number of bins (Figure 6).

Table 1 summarize results for the mixing index for fractal designs with different fractal dimensions (D = 1.25, 1.50 and 1.75) and SHB geometries with two different ridge spacings and an apex y – position range of ± 50 μm.

Design	Spacing 75 μm	Spacing 125 μm
D = 1.25	0.96	0.99
D = 1.50	0.96	0.99
D = 1.75	0.94	0.97
SHB	0.90	0.96

Table 1. Mixing indexes for an apex range of ±50 μm.

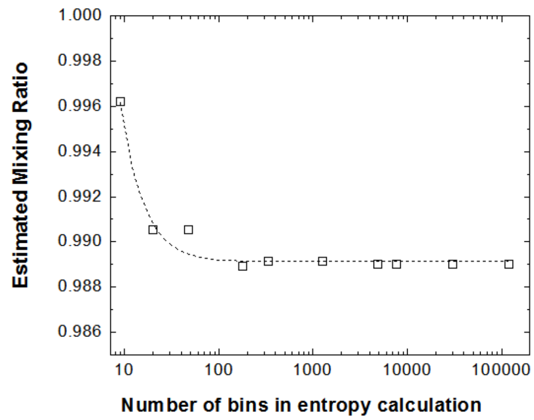

Figure 6. Dependence of the entropic measure on the number of bins used.

For all the spacing values the entropic measure of the mixing at the channel outlet is consistently better for the fractal designs for all the fractal dimensions used, when compared with SHB designs with the same geometrical parameters.

6. Conclusions

The COMSOL Multiphysics package was used to perform a computational assessment of the mixing efficiency of rectangular channels with slanted ridges patterned on the bottom surface. These geometrical structures have shown the ability to induce transversal flows, and thus increase the mixing quality. A mixing index based on entropy is used to quantify the mixing efficiency of different channels. The mixing quality is superior in fractal based designs, possibly due to the more chaotic flow associated with a system on which non-periodic boundary conditions are imposed.

7. References

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8. Acknowledgements

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