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Computations of Chaotic Flows In Micromixers

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Introduction: Microfluidic devices are important components of chemical and biological sensors proposed for many Naval and civilian applications. The problem of controlling fluid mixing in microdevices is often critical to their successful operation. This is especially true for cases involving chemical reaction, in which the reactants and products must be delivered to selected target locations within a specified concentration range. Flows in these devices are laminar (low Reynolds number), and mixing is controlled by the relatively slow process of molecular diffusion. An important practical issue is how to modify the flow to speed up the mixing process.

One method used to enhance mixing is surface patterning, in which structures are placed along one or more surfaces of a channel. Stroock et al.[1] have shown that repeating sequences of bas-relief herringbone-shaped structures on the floor of a microchannel create flow patterns that increase the interface area between the fluids to be mixed. The geometrical arrangement of obstacles stretches and folds the fluid, so that surface area between fluids is increased and mixing is enhanced. This phenomenon is called chaotic advection.

We are working on a joint computational and experimental effort to design and build microreactors with enhanced and controlled mixing and surface delivery capabilities. In the work described here, we have used numerical simulations to study chaotic advection and focus on the Stroock et al.[1] mixer. The numerical model[2] solves the three-dimensional incompressible Navier-Stokes equations coupled with an equation that describes the advection of a passive scalar, such as a marker dye.

Staggered Herringbone Mixer: Figure 6 shows the staggered herringbone configuration. This micromixer contains two full sequences of herringbone structures. Each sequence consists of six herringbones with the short segment on the left and the long segment on the right, followed by six more herringbones with the short segment on the right and the long segment on the left. At the inflow boundary, water enters at 1 cm/s, while the outflow boundary is set at a fixed pressure of 1 atm.

The major effect of the herringbone structures is to deflect the flow in such a way that the interface area between the fluids increases, and therefore mixing is enhanced. This flow pattern results in convective rolls in the cross section of the microchannel, as shown by the velocity vectors in Fig 6. For the first six herringbones, the larger convective roll is located on the right-hand side (the side with the longer segment), while the smaller convective roll is on the left-hand side (the side with the shorter segment). The flow is reversed for the second set of six herringbones, when the long and short segments of the herringbone structure have been switched.

Advection of Passive Scalars: To evaluate mixing effectiveness, two passive scalars, “red” and “purple,” are introduced at the inflow. The passive scalars follow the streamlines of the flow but have no interaction with the fluid, similar to a dye. Figure 7 shows images of the two passive scalars, at the indicated cross sec-

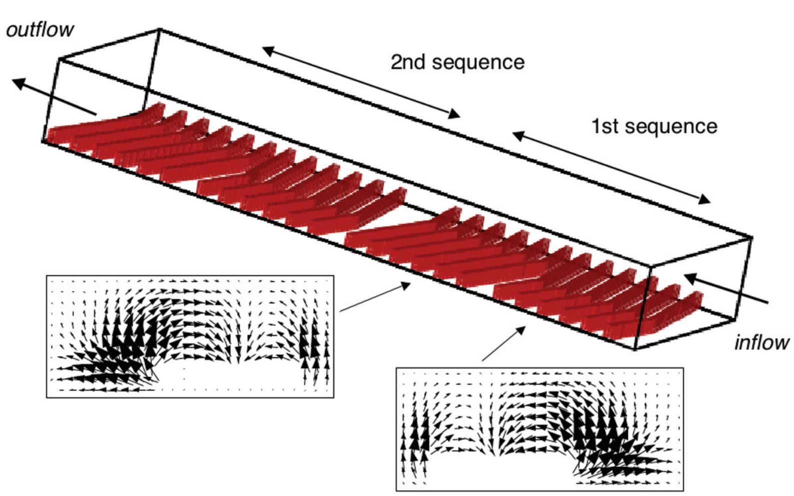

FIGURE 6
Schematic of staggered herringbone mixer. Dimensions are 90 × 200 μm in the cross section, and 4000 μm in length. Individual herringbones are 20 μm high. Velocity vectors show the convective rolls that are formed due to the herringbone structures.

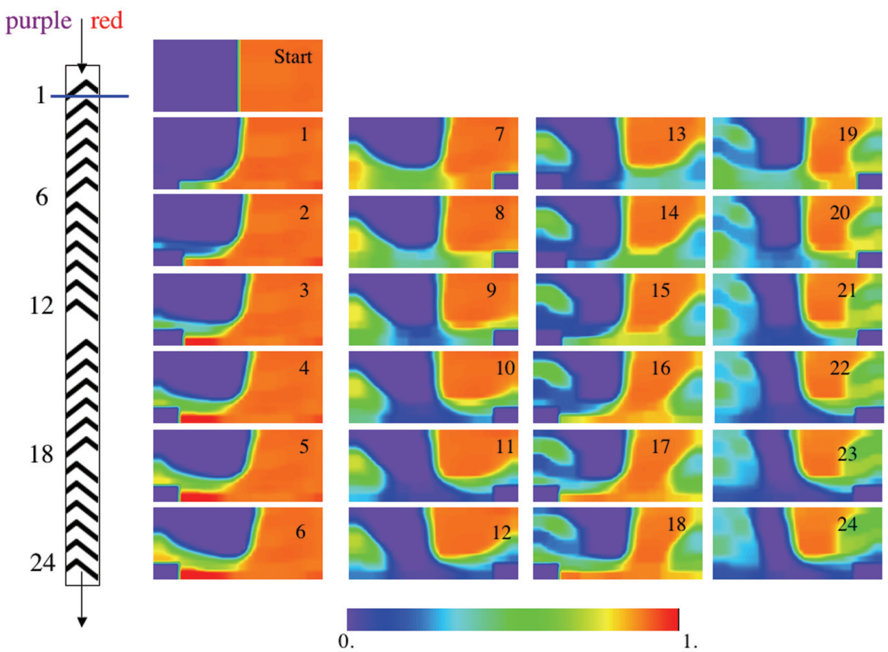

FIGURE 7
Mixing of two passive scalars in the staggered herringbone mixer.

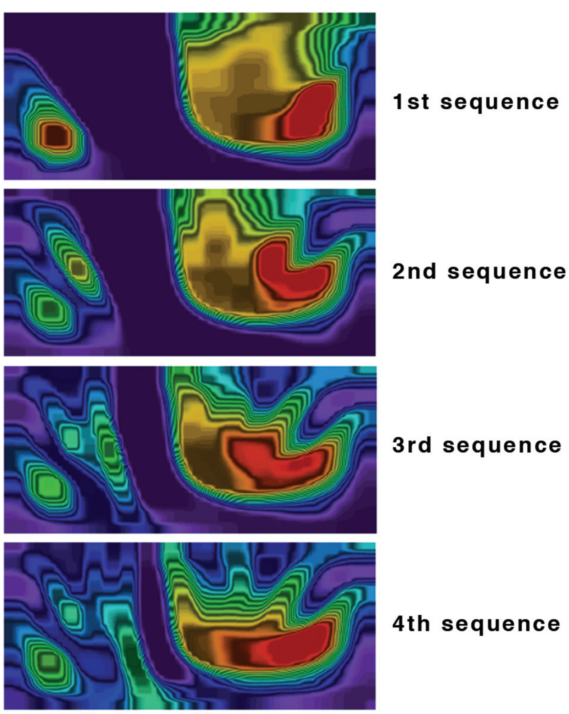

FIGURE 8
Calculations on a 3200 × 36 × 80 grid, using computational cells of 2.5 μm, that show stretching and folding indicative of chaotic advection after four sequences in the herringbone mixer.

tional planes. That is, "1" corresponds to the plane immediately after the first herringbone. Initially, at time zero, "red" fluid is on the right and "purple" fluid is on the left. For the first six herringbones, the larger convective roll forms on the left side. Therefore, purple fluid is pushed toward the right, near the top of the microchannel, while red fluid is pulled toward the left, near the bottom. When the herringbone pattern is reversed (structures 7 through 12), the red fluid is pushed upward and over to the left at the top, while purple fluid is pulled toward the right near the bottom. At the end of the first sequence of herringbones (after structure 12), some of the red fluid has travelled to the left side and some of the purple fluid has travelled to the right side, resulting in green fluid, which corresponds to well-mixed fluid. This flow pattern repeats itself during the second full cycle of structures, herringbones 13 through 24.

Chaotic Flow: Figure 7 shows that the resulting passive scalar concentrations become more complex after the second set of herringbones, compared to the first. In fact, in Stroock's mixer, which contains 15 full sequences of herringbones, the striations in the flow become finer with each successive herringbone sequence. To capture the finer scales of mixing that are indicative of chaotic advection, the resolution of the calculations must be increased. Figure 8 shows results for a high-resolution calculation containing four complete sequences of herringbone structures. This calculation shows how the flow becomes more complex and the striations become finer as the number of sequences increase.

Discussion: The term *chaotic advection* is used to describe a type of complex behavior that a passive scalar can show under specific conditions. It is an important phenomenon to understand and be able to use for controlling microflows. For a fluid to exhibit chaotic advection, it must be driven, folded, and stretched. In the flows shown here, the bending and stretching is accomplished passively, due to the herringbone structures. This leads to the formation of striations in the passive scalars, which become finer and finer as the flow develops. The result is an exponential increase in the surface area between the different fluids.

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[2] D.R. Mott, C.R. Kaplan, and E.S. Oran, "Development of a Robust Incompressible Solver for Cartesian Grids with Colocated Variable Arrangement," AIAA Paper No. 2004-0248, American Institute of Aeronautics and Astronautics, Reston, VA, 2004.