

Multiphysics Simulation of Chaotic Mixing in Microfluidic Devices

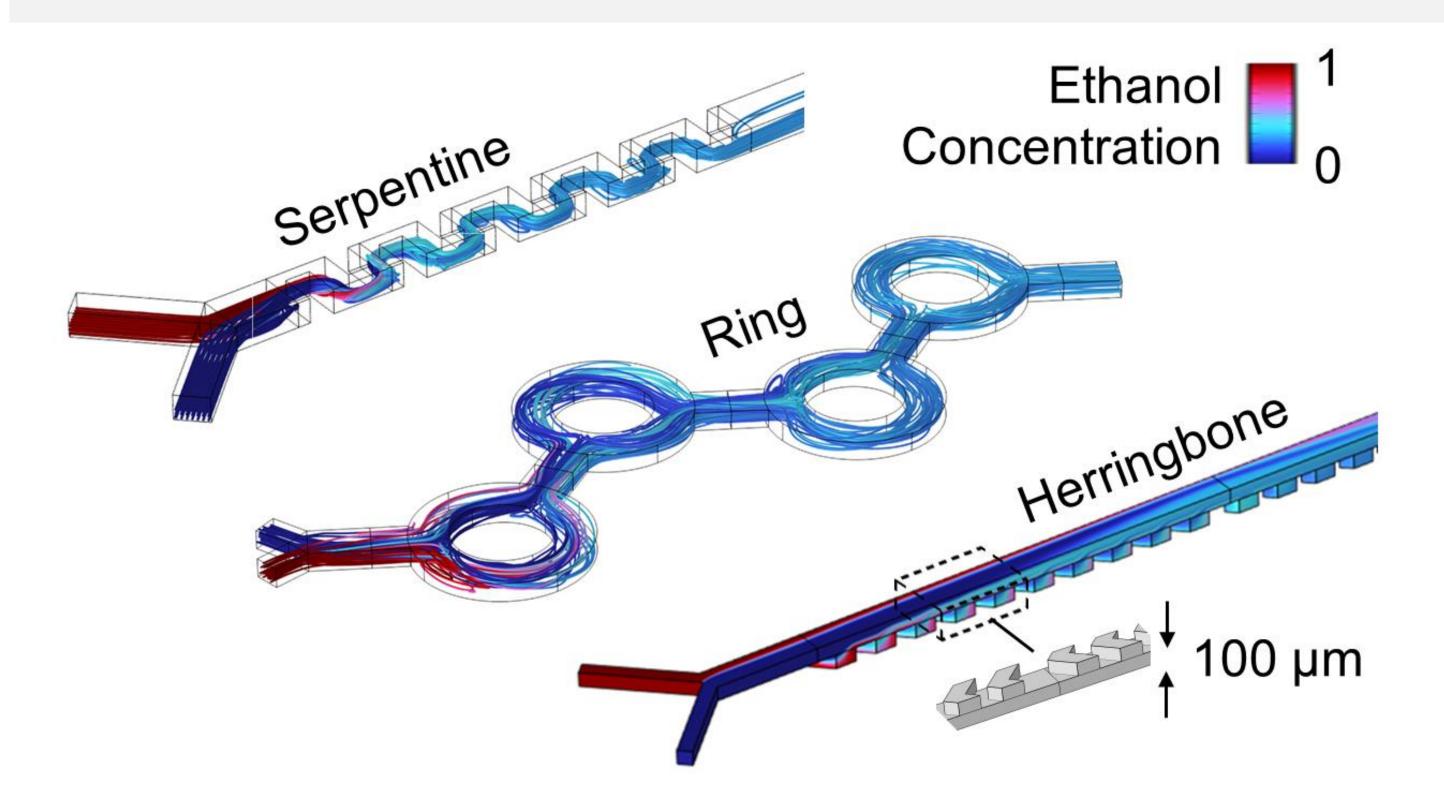
Prediction of flow and species transport in COMSOL Multiphysics[®] can inform design and operating parameters to maximize mixing efficiency and performance of microfluidic devices.

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Introduction

Fast mixing of reagents in microfluidic devices is important for DNA sequencing, small-batch mRNA vaccine production, and point-ofcare diagnostics. A key challenge in microfluidics is mixing reagents rapidly in a minimal amount of space. One way to do this is via chaotic mixing induced by geometrical features such as bends, turns, and grooves. In this study, we use computational fluid dynamics (CFD) simulations to evaluate the mixing of ethanol and water for three common microfluidic chaotic mixers (Figure 1). The serpentine mixer uses recirculation to achieve mixing. The herringbone mixer contains asymmetric grooves that cause the flow to stretch and fold exponentially with distance along the channel axis, independent of fluid inertia. The ring mixer employs Dean flows – vortices in the channel cross-section generated by centripetal acceleration of fluid elements. Simulations such as these help improve the design and performance of microfluidic mixers, thereby reducing development time and cost.



Methodology

Models of three microfluidic chaotic mixers were developed in COMSOL Multiphysics[®] with the Laminar Flow and Transport of Diluted Species

FIGURE 1. Three microfluidic mixers studied in this work. Flow streamlines are colored by ethanol mass fraction.

interfaces. Water and ethanol flowed into separate inlets in each device at specified flow rates. We used the concentration-dependent water-ethanol viscosity in the model: a 50/50 wt% water-ethanol mixture is more than twice as viscous as either pure component! We used separate meshes for flow and species transport; mesh resolution of each was optimized to ensure mesh converged results. Mixing efficiency was quantified by the mixing time, defined herein as the time required for the standard deviation of ethanol mass fraction over a channel cross section to be cut in half.

Results

Mixing visualizations shown in Figure 1 include streamlines colored by relative ethanol concentration by mass. The title figure samples the concentration distributions at various channel cross-sections in the serpentine mixer to visualize the degree of mixing, which increases progressively along the flow direction. Mixing time is plotted in Figure 2 for each device as a function of the Reynolds number, which is proportional to the flow rate. The serpentine and ring mixers demonstrate efficient mixing at high flow rates, due to strong fluid inertia. By contrast, the herringbone mixer exhibits short mixing times across a much broader range of flow regimes due to more efficient stretching and folding of fluid elements. In conclusion, these simulations can be used to design the geometry and inlet flow rates of microfluidic mixers to optimize their performance, thereby reducing development time and cost.

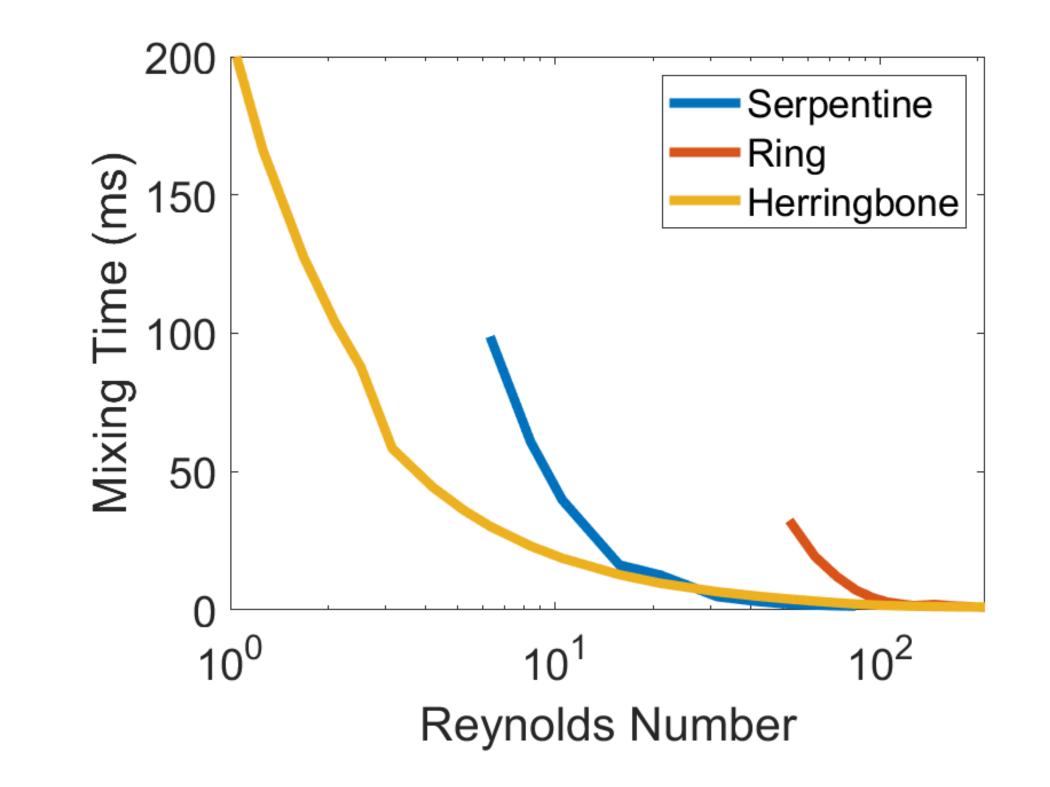


FIGURE 2. Comparison of mixing time vs. Reynolds number for prototypical microfluidic mixers.

REFERENCES

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- Spann AP, Hancock MJ, Rostami AA, Platt SP, Rusyniak MJ, Sundar RS, Ind. Eng. Chem. Res. 2021, 60, 670–677. <u>https://doi.org/10.1021/acs.iecr.0c00379</u>
- 3. For more details, visit <u>https://www.veryst.com/case-studies/chaotic-mixing-microfluidic-devices</u>



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