Performance Analysis of Herringbone Groove Patterns in microchannels for Passive Mixing.

ME 224, Microscale Flows

Submitted by

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Abstract

Microfluidic systems play a crucial role in biomedical diagnostics, chemical synthesis, and lab-on-chip devices, but they face a fundamental challenge: efficient mixing under laminar flow conditions. Due to the low Reynolds numbers and the dominance of viscous forces at the microscale, conventional turbulent mixing methods become ineffective. To overcome this limitation, we explored the use of herringbone microstructures, which induce chaotic advection and enhance passive mixing.

Drawing inspiration from two established designs—the bilayer staggered herringbone micromixer and convex groove configurations—we investigated the influence of groove geometries on mixing performance. Our study focused on two distinct microchannel designs: angular grooved channels and symmetric staggered herringbone channels. These microchannels were fabricated using soft lithography and analysed through both experimental and computational approaches. Experimental studies evaluated mixing efficiency, while numerical simulations in COMSOL 6.0 provided insights into flow behaviour by examining surface velocity distribution, concentration gradients, mixing length and vorticity.

The results demonstrate that carefully optimized groove geometries significantly enhance mixing efficiency by reducing the required mixing length and promoting chaotic advection. By leveraging these findings, this study offers valuable design strategies for improving microfluidic mixing performance in advanced applications.

Content

1. Introduction

Microfluidic devices play a critical role in chemical analysis, biomedical diagnostics, and lab-on-chip technologies due to their high precision, reduced reagent consumption, and enhanced process control. However, the inherently laminar nature of microfluidic flows severely limits mixing efficiency, as molecular diffusion remains the dominant transport mechanism. This constraint poses a significant challenge for applications requiring rapid and efficient mixing to facilitate biochemical reactions, analyte detection, and microreactor performance. Thus, improving passive micromixing strategies is essential for enhancing reaction kinetics and overall device functionality.

Among various passive mixing techniques, herringbone microstructures have emerged as a highly effective approach for inducing chaotic advection and secondary flow patterns without the need for external energy input. This study investigates two optimized herringbone geometries inspired by existing literature: **staggered bilayer herringbone structures** and **convex-concave herringbone configurations**. These designs leverage engineered surface patterns to generate transverse flow components and enhance interfacial stretching, thereby significantly improving mixing performance.

To systematically evaluate the effectiveness of these designs, a **dual-methodology approach** is adopted, incorporating both **experimental fabrication** via soft lithography and **computational fluid dynamics (CFD) simulations**. Two distinct microchannel architectures—**angular grooved channels** and **symmetric herringbone channels**—are analysed to assess their mixing efficiency. Critical flow parameters, including concentration gradients, velocity distribution, vorticity formation, and mixing length, are quantitatively examined to characterize their influence on micromixing dynamics.

By integrating experimental validation with high-fidelity numerical simulations, this study provides a comprehensive framework for the optimization of herringbone-based microfluidic mixing strategies. The findings contribute to the advancement of next-generation lab-on-chip devices, facilitating more efficient microfluidic processes for biomedical, pharmaceutical, and chemical applications.

2. Literature Review

1. **Bilayer Staggered Herringbone Micro-Mixer (SHM) [1]:**

   Bilayer staggered herringbone micromixers (BHM) have demonstrated significant improvements by leveraging structured asymmetry to induce **chaotic advection** and enhance transverse mixing.

   - **Objective:**
     Improve passive mixing efficiency by incorporating **asymmetric bilayer groove structures**, thereby inducing secondary rotational flows and reducing diffusion length.

   - **Methodology:**
     A dual approach combining **fluorescence microscopy experiments** and **CFD simulations (FLUENT® and COMSOL 3.5a)** to systematically analyse mixing performance.

   - **Key Design Parameters:**
     - **Channel Dimensions:** Length = 30 mm, Width = 200 µm, Depth = 200 µm.
     - **Herringbone Grooves:**
       1. **Angle:** 45° relative to the flow direction.
       2. **Depth:** 50 µm on both top and bottom surfaces.
       3. **Width:** 200 µm with an **inter-groove spacing** of 50 µm.
       4. **Asymmetry:** Major arm = 280 µm, Minor arm = 200 µm.

   - **Performance Indicators:**
     - **Mixing length:**
       Defined as the axial distance required to achieve 80% mixing.

     - **Fluorescence intensity:**
       Monitored to quantify interfacial diffusion and chaotic advection effects.

     - **Helicity and vorticity:**
       Used to evaluate secondary flow structures and rotational mixing patterns.

     - **Asymmetry index (AI):**
       Characterizes groove asymmetry, influencing rotational flow intensity.

   - **Findings:**

- Introducing bilayer herringbone structures with increasing **asymmetry index (AI = 1.4 to 2.0)** significantly **reduces the mixing length to approximately 6 mm**, compared to longer mixing lengths in conventional SHM designs.

- The formation of **multiple rotational centers** in asymmetric bilayer designs amplifies flow perturbations, enhancing **chaotic stretching and folding** of fluid layers.

- Numerical simulations confirm that **higher AI values increase helicity and x-vorticity**, reinforcing the role of **geometric asymmetry** in promoting rapid microfluidic mixing.

These results underscore the effectiveness of **bilayer herringbone microstructures** in optimizing passive micro mixing strategies, providing a **scalable and energy-efficient approach** for next-generation lab-on-chip applications.

2. Convex Grooves in Staggered Herringbone Mixers [2]:

- **Objective:**
  Investigate the impact of convex grooves on mixing efficiency by enhancing chaotic advection and reducing mixing length. The study compares convex and concave grooves to identify the optimal design for improved microfluidic mixing.

- **Methodology:**
  Mixing performance is analysed through **experimental validation** and **CFD simulations (FLUENT® and COMSOL 3.5a)**, using **fluorescence intensity measurements** and **flow field analysis** to evaluate the impact of **convex grooves** on chaotic advection.

- **Key Design Parameters:**

  - **Channel Dimensions:** Width = 200 µm, Depth = 90 µm.
  - **Groove Characteristics:**
    1. **Width:** 50 µm per groove
    2. **Depth:** 50 µm on top, bottom surfaces
    3. **Orientation:** 45° angle relative to downstream direction.

  - **Spacing & Cycles:**
    1. **Cycle Spacing:** 500 µm per cycle
    2. **Repetition:** 10 cycles in total

- **Performance Indicators:**

- **Mixing Efficiency:**
  Measured via fluorescence intensity to assess homogeneity.

- **Number of Mixing Cycles:**
  Determined by the mixing length (distance for 80% mixing).

- **Flow Patterns:**
  Evaluated using helicity and vorticity to analyse rotational mixing.

- **Reynolds Number:**
  Laminar regime ($Re < 1$) validates geometric effects, including asymmetry index (AI) on flow intensity.

- **Findings:**

  - **Convex groove designs** achieve approximately **twice the mixing efficiency** compared to concave configurations, highlighting the superior performance of convex geometries.

  - The **flow patterns** in convex grooves generate stronger **vortices and rotational structures**, which enhance chaotic advection and improve mixing.

  - Convex grooves achieve **complete mixing in just 2 cycles**, whereas concave grooves require **4–5 cycles**, demonstrating their efficiency.

  - Operating in the **laminar regime ($Re < 1$)**, convex grooves leverage geometric modifications to optimize passive mixing without external turbulence (active mixing means).

The findings demonstrate the significant advantages of convex grooved herringbone microstructures in enhancing passive micro-mixing, providing a scalable and energy-efficient platform for advanced lab-on-chip systems. Their superior performance underscores their potential for practical applications in microfluidics.

3. Motivation and Objective

Motivation:

Microfluidic devices operate predominantly in the **laminar flow regime**, where mixing is constrained by slow **molecular diffusion**. This limitation often leads to **inefficient mixing**, which can significantly hinder reaction rates and reduce the overall performance of applications such as **chemical analysis**, **biomedical diagnostics**, and **lab-on-chip systems**. Efficient mixing is not just desirable but **essential** for enhancing **reaction speed**, **measurement accuracy**, and the **functionality** of these devices. While **active mixing techniques**—such as electromagnetic, acoustic, or pressure-driven methods—can improve mixing, they come with drawbacks, including the need for **external power sources** and **complex control mechanisms**. In contrast, **passive mixing** offers a **simpler**, **energy-free alternative** by leveraging modifications in channel geometry to induce **chaotic advection** and secondary flows. Among passive mixing strategies, **herringbone-grooved microchannels** have proven to be particularly effective. Their unique design disrupts laminar flow, creates vortices, and enhances mixing even at **low Reynolds numbers**, making them ideal for microfluidic applications. This project seeks to **explore** and **optimize** herringbone-grooved microchannels, addressing the pressing need for **efficient**, **scalable**, and **energy-free mixing solutions** in next-generation microfluidic systems.

Objective

The primary objective of this study is to systematically evaluate the mixing performance of microfluidic channels incorporating **herringbone microstructures**, with the goal of optimizing passive mixing efficiency. This research aims to bridge the gap between experimental observations and computational fluid dynamics (CFD) simulations, providing insights into the role of groove geometry in enhancing chaotic advection. The specific objectives are as follows:

- **Comparative Analysis:** Conduct a **quantitative assessment** of four distinct microchannel configurations—**straight channels (control), vertical grooves, angular staggered grooves, and symmetric staggered herringbone grooves**—to determine the influence of groove geometry on mixing efficiency. Key performance indicators include **mixing length, concentration distribution, and flow perturbations**.

- **Design Optimization:** Identify **geometric and structural parameters** (e.g., groove depth, width, spacing, and asymmetry index) that minimize mixing length while maximizing **chaotic advection-induced fluid interdiffusion**. The study aims to establish optimal design principles for enhancing passive micro mixing in low-Reynolds-number flows.

- **Fabrication Methodology:** Develop and refine **soft lithography techniques** for high-fidelity microchannel fabrication, addressing key challenges such as **mould accuracy, feature replication, PDMS curing uniformity, and bonding integrity** to ensure reproducibility and structural precision.

- **Computational and Experimental Correlation:** Utilize **CFD simulations (COMSOL Multiphysics)** to analyse **velocity fields, vortical structures, helicity, and vorticity distributions**, validating experimental findings and providing deeper insights into the flow dynamics governing micro mixing.

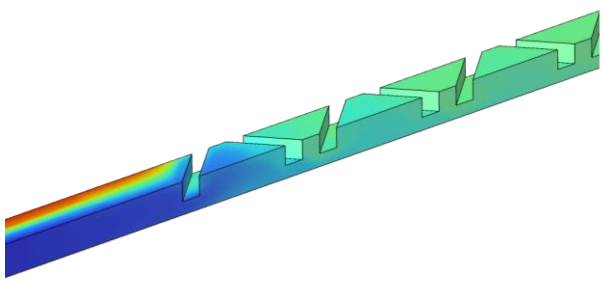
By accomplishing these objectives, this study aims to advance the design and optimization of **energy-efficient, high-performance microfluidic mixers** for applications in **biochemical assays, lab-on-chip devices, and point-of-care diagnostics**.

4. Methodology

The methodology for this project is divided into four main sections: **Experimental Procedure and Microchannel Fabrication**, **Experimental Results and Mixing Procedure Evaluation**, **Computational Fluid Dynamics (CFD) Simulation**, and **Data Evaluation from CFD Simulation**. Each section is designed to ensure a systematic approach to analysing and optimizing passive mixing in herringbone-grooved microchannels.

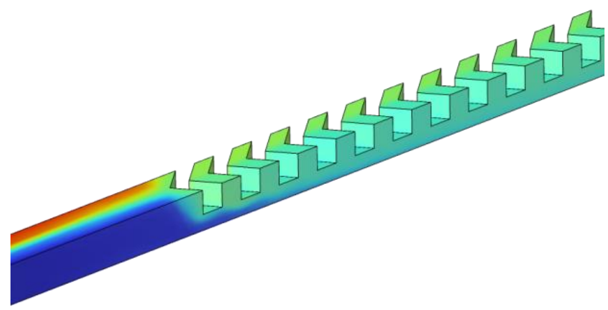
1. Experimental Procedure and Microchannel Fabrication

Microchannel Design



Angular Grooved Channel:
Channel Dimensions: Width = 200 µm, Depth = 200 µm.

Groove Specifications: Depth = 120 µm, Groove Angle = 45°, Spacing = 100 µm, Width = 100 µm.



Symmetric Herringbone Channel:
Channel Dimensions: Width = 200 µm, Depth = 200 µm.

Groove Specifications: Depth = 120 µm, Groove Angle = 90°, Spacing = 100 µm, Width = 100 µm.

Fabrication Process

The fabrication process involved the following steps:

- **Modelling and Mold Printing:**
  High-resolution moulds for both microchannel geometries **(Angular Staggered Grooves and Symmetric Staggered Herringbone Grooves)** were designed and printed.

- **Mold Cleaning and Characterization:**
  Molds were cleaned using **isopropyl alcohol (IPA)** and their dimensions were verified for accuracy.

- **PDMS Preparation:**
  Polydimethylsiloxane (PDMS) was mixed with a curing agent in a **10:1** ratio and degassed to remove air bubbles.

- **Casting and Curing:**
  PDMS was poured into the moulds and cured at **60°C for 5 hours and 30 minutes.** The cured PDMS was carefully peeled off from the moulds.

- **Glass Slab Preparation and Bonding:**
  Glass slides were cleaned with IPA, spin-coated with PDMS **(5:1 ratio),** and bonded to the PDMS microchannels. The assembly was baked at **60°C for 1 hour** to ensure strong bonding.

- **Microchannel Testing:**
  Inlet and outlet holes were punched, and the microchannels were connected to a syringe pump operating at a flow rate of **0.5 mL/min.** Flow behaviour was observed to ensure proper functionality

2. Experimental Results and Mixing Procedure Evaluation

- **Objective**

  - **The experimental phase aimed to:**
    - Analyse passive mixing in **angular grooved** and **symmetric herringbone-grooved** microchannels.

    - Evaluate **concentration gradients** and **normal velocity** at different sections of the channel **(front, middle, and back).**

- **Validation of Experimental Results**

Experimental results are to be validated through:

- **Visual Inspection:**
  The **concentration distribution** of two fluids (e.g., blue dyed and red dyed solutions) was visually observed to assess mixing efficiency.

- **Mixing Length Measurement:**
  The distance required to achieve complete mixing **(mixing length)** was measured and compared for both microchannel designs.

- **Outcome**
  The experimental results identified which groove configuration achieved **better mixing over a shorter distance**, providing a basis for further optimization.

3. Computational Fluid Dynamics (CFD) Simulation

- **Simulation Setup**
  - CFD simulations were performed using **COMSOL Multiphysics** to analyse fluid behaviour in the microchannels. The following parameters were defined:
  - **Boundary Conditions**:
    - **Inlet:** Two fluids with initial concentrations of 50 mol/m³.
    - **Inlet Flow Rate**: 0.499 mL/min.
    - **Outlet:** Pressure = 0 Pa (gauge pressure).
    - **Diffusion Coefficient:** 2.3×10^{-9} m²/s. [3]
  - **Flow Regime:** Laminar flow (Reynolds Number, Re = 41.5).

- **Analysis Performed**

  - **Velocity Distribution:**
    Examined at the **front, middle, and back** sections of the channel to understand flow disturbances and vortices.

  - **Concentration Gradient:**
    Tracked the progression of mixing along the channel length.

  - **Mixing Length:**
    Determined for both microchannel designs to compare their **mixing efficiency.**

4. Data Analysis from CFD Simulation

- **Objective**

- The CFD simulation data was evaluated to:
  Compare the **mixing efficiency** of **angular grooved** and **symmetric herringbone-grooved** microchannels.

- Validate experimental results by correlating simulated **concentration gradients** and **mixing lengths** with experimental observations.

- Key Metrics

  - **Velocity Profiles:**
    Analysed to identify regions of **high vorticity** and **chaotic advection**.

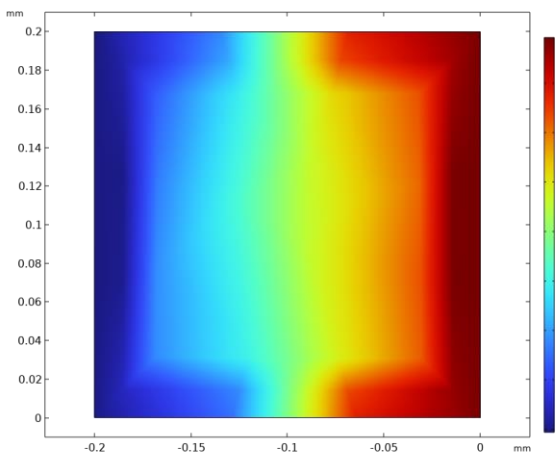
  - **Concentration Profiles:**
    Used to quantify **mixing efficiency** and determine the **mixing length.**

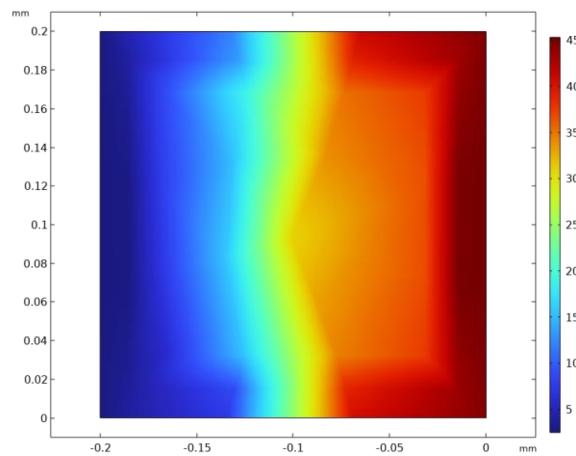
  - **Mixing Efficiency:**
    Calculated based on the **homogeneity of concentration distribution** across the channel.

- Outcome
  The CFD simulations provided insights into the **flow patterns and mixing mechanisms**, confirming the experimental findings and highlighting the superior performance of one groove configuration over the other.

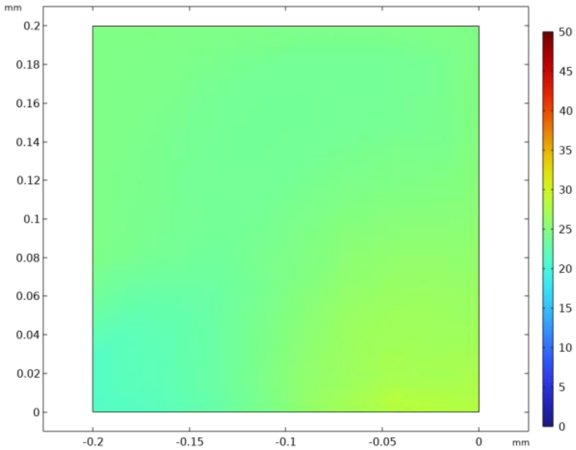
5. Results and Discussion

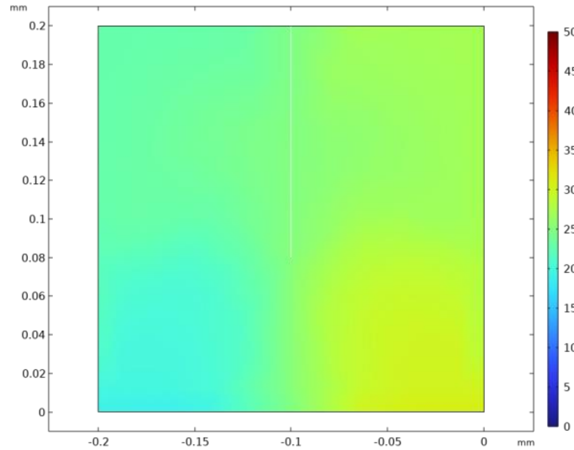
In the following section, we present a **comparative analysis** based on computational results obtained from **COMSOL Multiphysics 6.0**. The **Angular Herringbone Structure (AHS)** is shown on the **left**, while the **Symmetric Herringbone Structure (SHS)** is displayed on the **right**, allowing for a direct evaluation of their respective mixing performances.



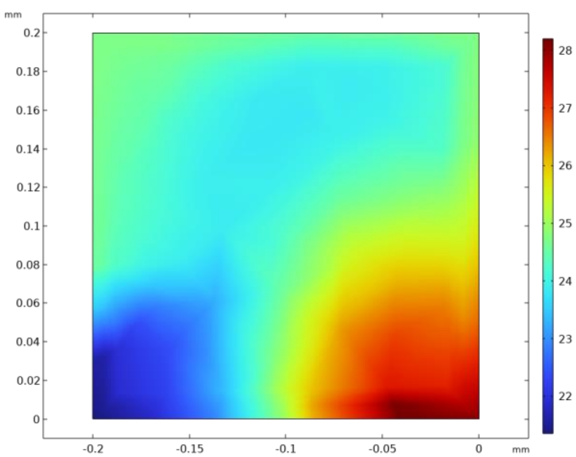


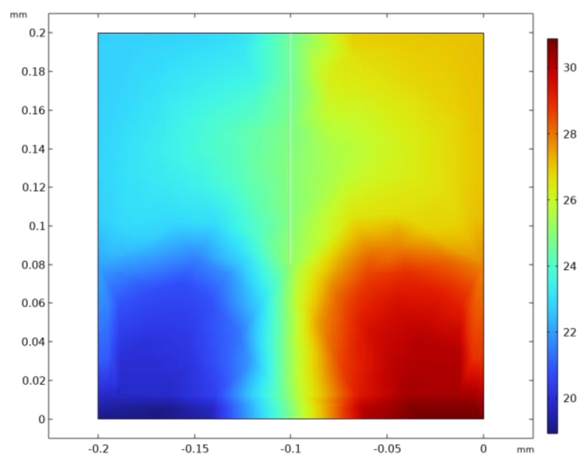
The concentration plots for both **AHS** and **SHS** presented above correspond to the fluid state immediately before the onset of the mixing process. These plots illustrate the concentration distribution of **Species 1**, where a lower concentration of Species 1 can be equivalently expressed as **(50 - C_1)**, representing the concentration of **Species 2**. This inverse relationship arises from the initial condition, where the total concentration of both species is maintained at **50 mol/mm^3**. This approach allows for a direct comparison of concentration gradients and mixing efficiency between the two microchannel designs.



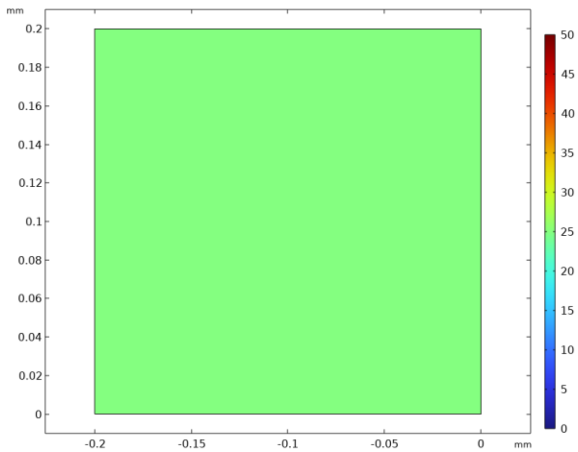


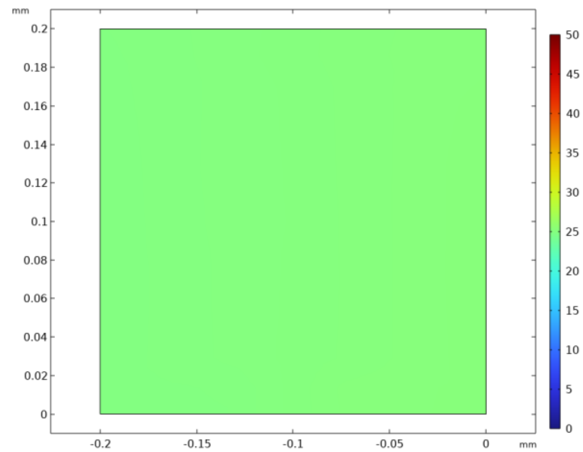
The concentration plots for both **Angular Herringbone Structure (AHS)** and **Symmetric Herringbone Structure (SHS)** shown above correspond to a position approximately **5.5 mm downstream** from the junction of the two inlets. At this stage, the two species have achieved **near-uniform mixing**, though complete homogeneity has not yet been attained. A comparative analysis indicates that **AHS exhibits a more uniform concentration distribution** compared to SHS, suggesting **enhanced mixing efficiency** due to its geometric influence on chaotic advection and fluid interdiffusion.



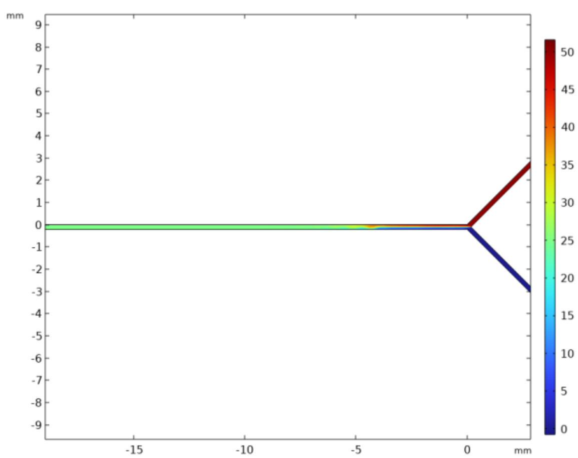


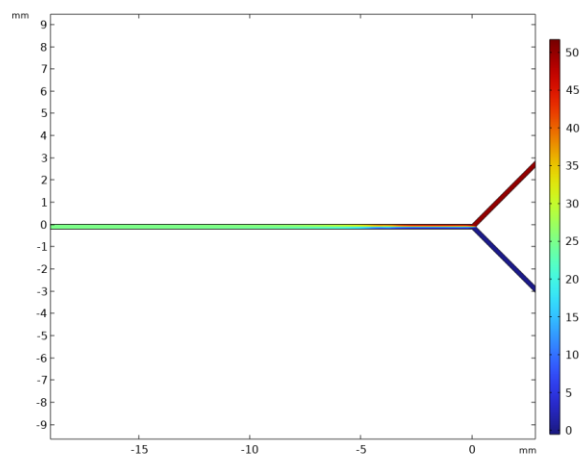
Closer examination confirms that **AHS achieves higher mixing efficiency**, with **C_1 ranging from 22–28 mol/mm^3**, compared to **20–30 mol/mm^3 in SHS**. The narrower range in AHS indicates more uniform species distribution and enhanced mixing performance.



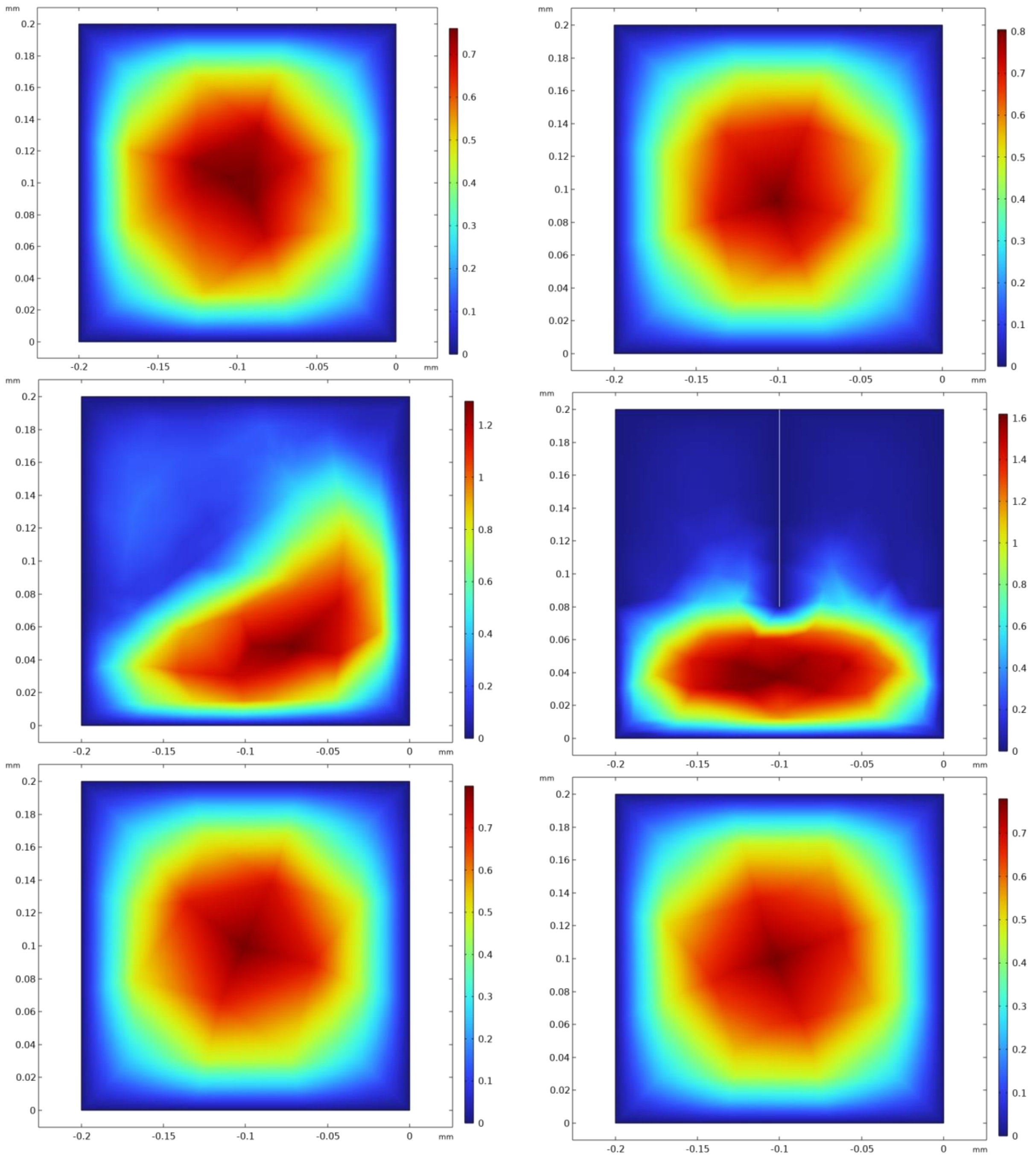


After passing through the mixer, both **AHS** and **SHS** achieve a **homogeneous distribution** of species within their respective channels, indicating effective mixing in both designs.

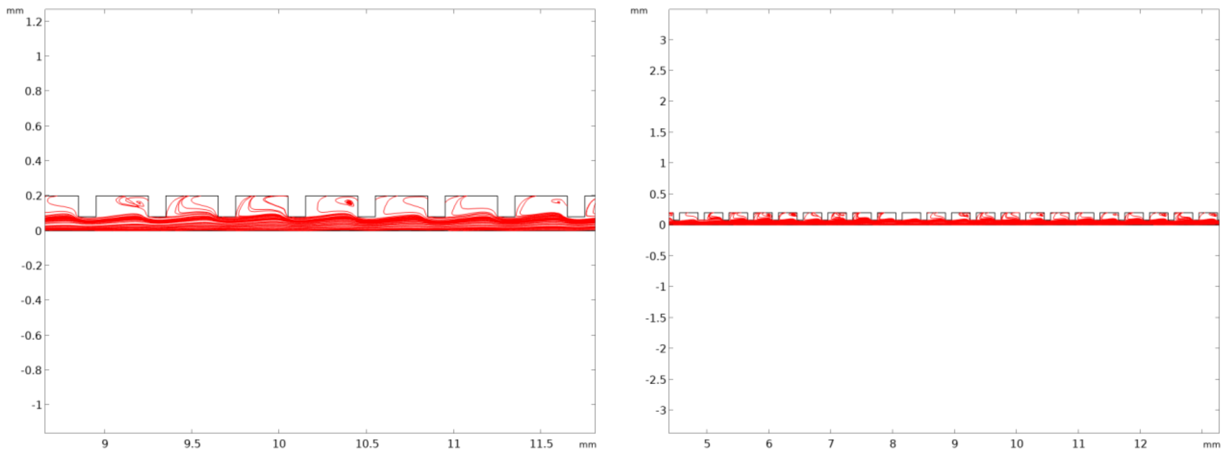




The above image illustrates the **final concentration distribution** after mixing, where **AHS achieves efficient mixing within 6 mm**, while **SHS requires 8 mm** to reach a comparable level of uniformity. This indicates **faster mixing performance** in AHS due to its enhanced chaotic advection.



The three images above depict the **velocity surface distribution plots** at **three key instances**: **during onset, at 5.5 mm, and after mixing**. These plots highlight the **unique flow characteristics** across the grooves, showcasing distinct velocity patterns that influence the mixing process.



The images illustrate the velocity streamlines for both the **SHS** and the **AHS**. Notably, AHS exhibits larger and more pronounced vortex formations, leading to enhanced chaotic advection and improved mixing efficiency. In contrast, SHS shows smaller vortices with less intense recirculation, indicating a more gradual mixing process. The distinct flow patterns highlight the superior mixing performance of AHS over SHS.

6. Challenges Faced

During the fabrication and experimental phases of the project, several challenges were encountered, which impacted the quality and performance of the microchannels:

1. **Groove Formation on the Top Surface**:
   During the **PDMS preparation** and **bonding with the glass slide**, the grooves were unintentionally formed on the **top surface** of the channel. This resulted in an **unobstructed flow path** for the fluids, preventing the generation of **turbulence** and significantly reducing mixing efficiency.

2. **Under curing of PDMS**:
   In some cases, the **PDMS was under cured**, causing it to **stick to the mould surface** when peeled off. This led to **incomplete or damaged channels**, which were not suitable for testing. Under curing often occurred due to **premature peeling** or insufficient curing time. The presence of **residual PDMS** between the grooves, caused by incomplete curing, further obstructed the flow path and hindered the formation of **secondary flow structures** necessary for effective mixing.

3. **Limitations in Fabricating Small-Scale Features**: The initial design of staggered herringbone structures with an inter-groove **spacing of 40 µm** could not be fabricated due to the limitations of the soft lithography technique. This restricted the ability to achieve **finer geometric features**, which are critical for enhancing **mixing efficiency.**

4. **Experimental Limitations**:
   Fluorescence-based experiments using blue and yellow dyes revealed **no significant mixing**, contradicting the expected results from **CFD simulations**. This discrepancy highlighted the impact of fabrication defects on the overall performance of the microchannels.

These challenges underscored the importance of **precise fabrication techniques** and **optimal curing conditions** to ensure the successful development of functional microchannels for passive mixing applications.

7. Conclusions

This study investigated the effectiveness of herringbone microstructures in enhancing passive micromixing within microchannels. Through a combination of experimental fabrication and computational fluid dynamics (CFD) simulations, we evaluated the performance of angular grooved and symmetric herringbone microchannel designs. The results demonstrated that the angular herringbone structure (AHS) exhibited superior mixing efficiency compared to the symmetric herringbone structure (SHS), achieving complete mixing within a shorter distance.

Key findings indicate that the optimized groove geometry in AHS generated stronger vortices, promoting chaotic advection and reducing the required mixing length. The experimental validation aligned well with simulation results, reinforcing the role of geometric modifications in improving mixing performance. The insights gained from this stuy offer valuable guidelines for the design of efficient microfluidic mixers, particularly in biomedical diagnostics, chemical synthesis, and lab-on-chip applications.

By leveraging passive mixing strategies such as herringbone microstructures, microfluidic systems can achieve enhanced mixing without external energy input, making them more efficient and scalable for real-world applications. Future work could focus on further optimizing groove parameters, exploring multi-phase flows, and integrating these designs into practical lab-on-chip devices for advanced microfluidic applications.

8. Future Scope

This study has demonstrated the effectiveness of herringbone groove structures in enhancing passive micromixing; however, several fabrication challenges remain that must be addressed to improve reproducibility and structural integrity. A key limitation encountered was the inability to fabricate bilayer grooves using soft lithography, restricting the induced chaotic advection to a single surface of the microchannel. Additionally, the grooves, being suspended from the mold, exhibited a propensity for tearing during the demoulding process, which compromises the precision and repeatability of the fabricated structures.

To mitigate these challenges, future research will focus on optimizing the soft lithography process to enhance the durability and reliability of the fabricated microchannels. Specifically, improvements in **PDMS curing protocols** will be implemented, including precise control over curing temperature and duration to prevent under curing, which can lead to weak structural integrity. Additionally, thorough degassing of PDMS before curing will be ensured to eliminate air entrapment, which may otherwise introduce structural defects. The use of **mold surface treatments**, such as silanization or alternative release coatings, will also be explored to facilitate smoother PDMS detachment, thereby minimizing mechanical stress on the grooves and reducing tear-induced defects.

Moreover, insights from existing literature will be leveraged to explore alternative **geometric modifications** that enhance mixing efficiency while remaining manufacturable within current fabrication constraints. Potential design modifications include variations in **groove depth, spacing, and orientation**, which could provide a balance between structural stability and effective chaotic advection. Computational fluid dynamics (CFD) simulations will continue to play a critical role in refining these designs prior to experimental validation, allowing for an informed selection of geometries that maximize mixing performance while ensuring fabrication feasibility.

By integrating these improvements in fabrication methodology and structural design, future work aims to develop more robust and reproducible microfluidic architectures. These advancements will contribute to the broader goal of enhancing passive micromixing strategies for lab-on-chip technologies, biomedical diagnostics, and chemical processing applications, thereby expanding the practical applicability of microfluidic systems.

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