Studying Diffusion and Fluid flow for gradient Formation in microfluidic platforms

ME224,Fundamental of

Microscale Flows

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Abstract

- Microfluidic systems enable precise manipulation of fluids at the microscale, making them indispensable for biomedical, chemical, and analytical applications. These systems play a critical role in lab-on-a-chip technologies, where controlled gradient formation is essential for processes such as drug screening, cell migration studies, and chemical synthesis. This study focuses on the design, simulation, and fabrication of a serpentine microfluidic mixer optimized for gradient generation by mixing two inlet streams of red and blue fluids, resulting in a controlled concentration gradient.

- Computational simulations were conducted using ANSYS Fluent to analyze flow behavior and diffusion characteristics. The Eulerian mixture model was employed to simulate laminar flow and species transport, incorporating Fick's Law to evaluate diffusion dynamics. The device was then fabricated using soft lithography with PDMS, ensuring compatibility with biological and chemical applications. Experimental validation was performed by injecting dyes at controlled flow rates to visualize gradient formation.

- The results demonstrated efficient and uniform gradient formation, with numerical and analytical hydraulic resistance values showing close agreement, with a 6.09% error. The study also observed anomalous diffusion effects, indicating non-ideal mixing characteristics. Additionally, velocity-dependent gradient control was identified, suggesting that adjusting flow rates can fine-tune gradient profiles. These findings contribute to the optimization of microfluidic mixing strategies, offering improvements for biomedical applications such as tissue engineering, targeted drug delivery, and high-throughput chemical screening.

Content

1. Introduction

Microfluidic systems are widely used for controlled fluid handling in biomedical, chemical, and analytical applications. These platforms enable precise control over chemical gradients, crucial for applications such as drug screening, tissue engineering, and chemical analysis. In biomedical research, gradient generators are essential for cell migration studies, morphogen gradient analysis, and high-throughput screening of drug responses. Chemical and material science applications also benefit from microfluidic gradient generators by enabling controlled reactions, nanoparticle synthesis, and localized surface modifications.

The challenge in microfluidic gradient generation lies in the interplay between advection and diffusion, governed by the Peclet number. When diffusion dominates, gradients form slowly, requiring longer microchannels. Conversely, when advection dominates, gradients may not develop uniformly, necessitating specialized channel designs such as serpentine structures, tree-shaped networks, and membrane-based diffusers. The precise design of these systems must account for factors such as Reynolds number, flow rates, and species transport dynamics to achieve desired gradient profiles.

This project aims to develop a serpentine microfluidic mixer optimized for controlled gradient formation. By leveraging computational fluid dynamics (CFD) simulations and experimental validation, we analyze how mixing efficiency and diffusion dynamics impact gradient uniformity. The ultimate goal is to enhance the performance of lab-on-a-chip systems, providing reliable and scalable solutions for biomedical and chemical applications. The integration of numerical simulations with experimental validation ensures an in-depth understanding of the microfluidic system's behavior, contributing to the ongoing advancements in microfluidic technology.

2. Literature Review

2.1. Generation of Solution and Surface Gradients Using Microfluidic Systems-by Noo Li Jeon, Stephan K. W. Dertinger

Introduced a microfluidic system that generates precise gradients using controlled mixing of laminar flows in microchannels.This system creates gradients by splitting, mixing, and recombining fluid streams. It can produce static gradients (fixed profiles) or dynamic gradients (adjustable profiles by changing flow rates).

2.2. Concentration gradient generation methods based on microfluidic systems -by Xiang Wang , Zhaomiao Liu * and Yan Pang

Different type of Gradient generators in Microfluidics with there respective advantages and disadvantages Namely-

- Tree Shape Networks - Network involving branching and recombining streams to create gradient
- Altered Tree Shape Network - Modified tree-shape networks aim to reduce limitations of traditional designs.
- Y Shape Junctions - generates gradients through molecular diffusion between streams.
- Membrane system - use porous materials to seperate flowing streams from the gradient chamber
- Pressure Balance system - these systems balance inlet and outlet pressures to elimination convection in gradient chamber

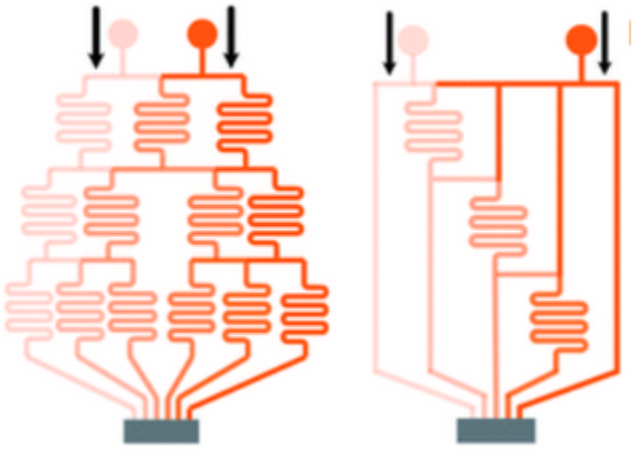

Fig 1 : Types of MicroFluidic Gradient generators

3. Motivation and Objective

3.1. Motivation:

Motivation behind this project is that Microfluidic systems are essential in biomedical and chemical research, enabling precise fluid control for applications like drug screening, tissue engineering, and chemical analysis. Efficient gradient formation is critical for these processes, requiring a deep understanding of diffusion and fluid flow dynamics in microchannels. This project aims to enhance microfluidic design for optimized gradient generation, contributing to advancements in lab-on-a-chip technology and controlled chemical mixing.

3.2. Objective:

- Investigate diffusion and flow dynamics in microfluidic platforms to improve gradient formation.
- Design and simulate a serpentine microfluidic gradient mixer using ANSYS Fluent.
- Fabricate the device using soft lithography techniques and validate its performance through experimental testing.
- Compare numerical and experimental results to assess the accuracy and efficiency of the proposed design.

4. Methodology

- Research Phase - Papers were reviewed on gradient formation to understand diffusion dynamics and microfluidic mixing strategies
- Cad modeling - The microfluidic mixer features three serpentine channels with two inlets for red and blue fluids. A single outlet allows observation of the resulting purple gradient formation with Total length - 31.75 mm and 40 mm by 47 mm Mold
- Simulation
    - Simulation on Ansys Fluent 2024 R1
    - We used the Eulerian mixture model for laminar flow (Re<1). Continuity , Momentum equations solved and Species Transport to apply Fick's law of diffusion.
    - Boundary Conditions
        - Inlet Velocity
        - Gauge Pressure = 0 along with no shear
- Fabrication
    - Soft Lithography
    - The resin mold was fabricated, cleaned, and cured. PDMS was poured, baked, peeled off, and bonded to a glass plate.
- Experimenting
    - Preparation of Dyes: Two separate dye solutions, red and blue, were prepared.
    - Injection into Inlets: The dyes were carefully poured into their respective microfluidic inlets.A volume flow rate of 0.2ml/min was set.
    - Gradient Formation: As the fluids traveled through the serpentine channels, controlled mixing occurred.

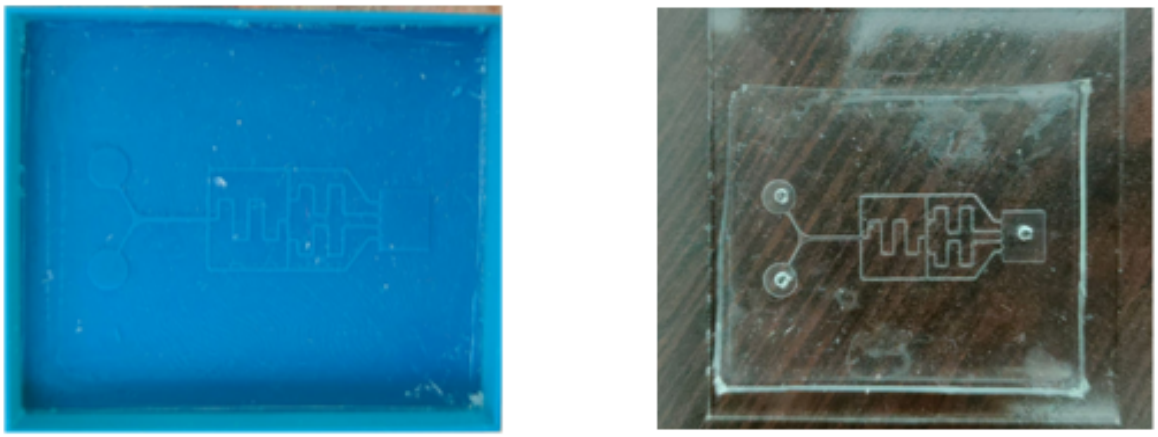

Fig 2 : Photographs of Mold and Microfluidic device

5. Results and Discussion

- ## Calculation:

Hydraulic Diameter Dh: where A = Cross Section and P is wetted perimeter

Dh = 4A/P = 204.87 microns

Reynolds Number:

Re = ρvDh/μ = 0.02 (indicating laminar flow)

Peclet Number:

Pe = Dhv/D = 205 (suggesting advection dominance over diffusion)

For water, the diffusivity D is 10^-10 m2/s.

- ## Numerical Simulation:

In Base case (Both Inlets have velocity of 1e-4m/s).Overall a uniform Gradient is obtained,which ensures the mixing is proper and uniform inside the serpentine channels

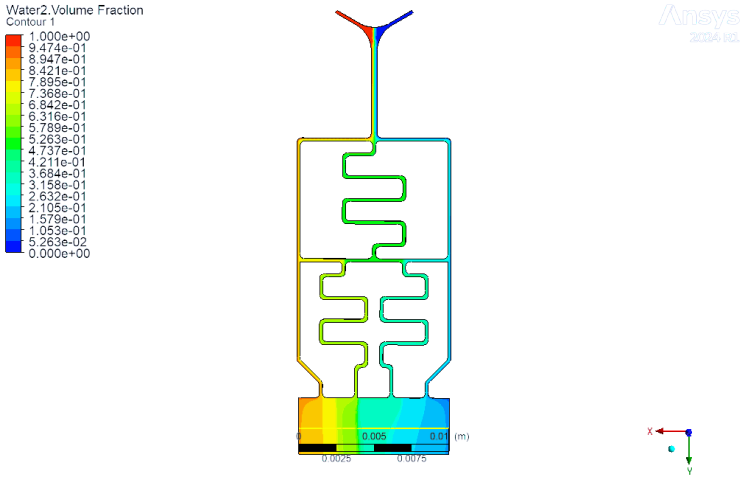

Fig 3: Simulation result

The volume fraction at the neck shows proper diffusion in the beginning of microfluidic devices. Also considered steady so by ficks law the gradient of concentration should be constant (C = ax + b). **Anomalous DIffusion** - as the concentration gradient is not perfectly linear and has some deviation with X.

The numerical pressure difference was calculated as 0.673 Pa with a velocity of 6.95×10^{-5} m/s in the branch.The numerical flow rate(Q) was determined to be 2.919×10^{-12} m^3/s.
The numerical hydraulic resistance was 2.09×10^{8} $Pa \cdot s/m^3$, while the analytical value was

(28 mu L/h^4)
Rh = 28*10^-3*12.22*10^-3/(204*10^-6)^4
Rh = 1.97×10^{8} $Pa \cdot s/m^3$

The error between numerical and analytical solutions was (2.09-1.97/1.97)*100 = 6.09%

Velocity Ratio= 1:2 Case (Inlets have velocity of 5e-5 m/s and 1e-4 m/s respectively)
A uniform gradient was observed for the red dye due to its higher velocity. This indicates that *achieving a low-slope gradient requires increasing the flow rate of the respective fluid.*

The distance of interface and wall is given by d(Q2/(Q1+Q2)).

In the Base Case, velocity Ratio is 1:1.
Q2=Q1
Thickness = d/2 where d= 400 microns
Thickness = 200 microns

In the Second Case, velocity Ratio is 1:2.
Q2=4Q1
Thickness=4d/5 where d= 400 microns
Thickness = 320 microns

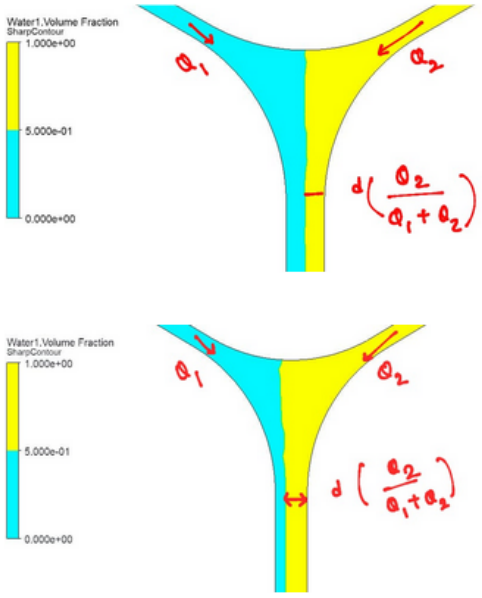

Fig 4: Interface Distance

- # Experimental calculation:

  Mixing of red and blue coloured dyed water and observing the gradient formation.Not much information is gathered from experiment as the intensities of the dye are too low.

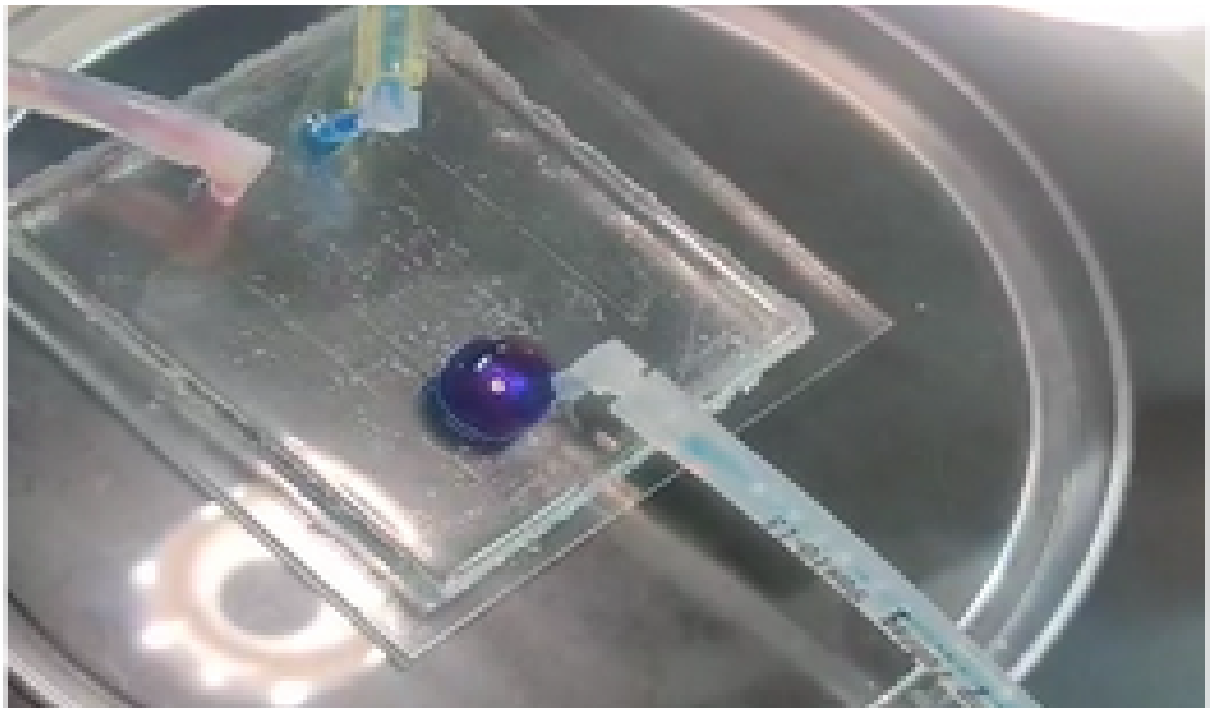

Fig 5: Outlet has violet coloured dye

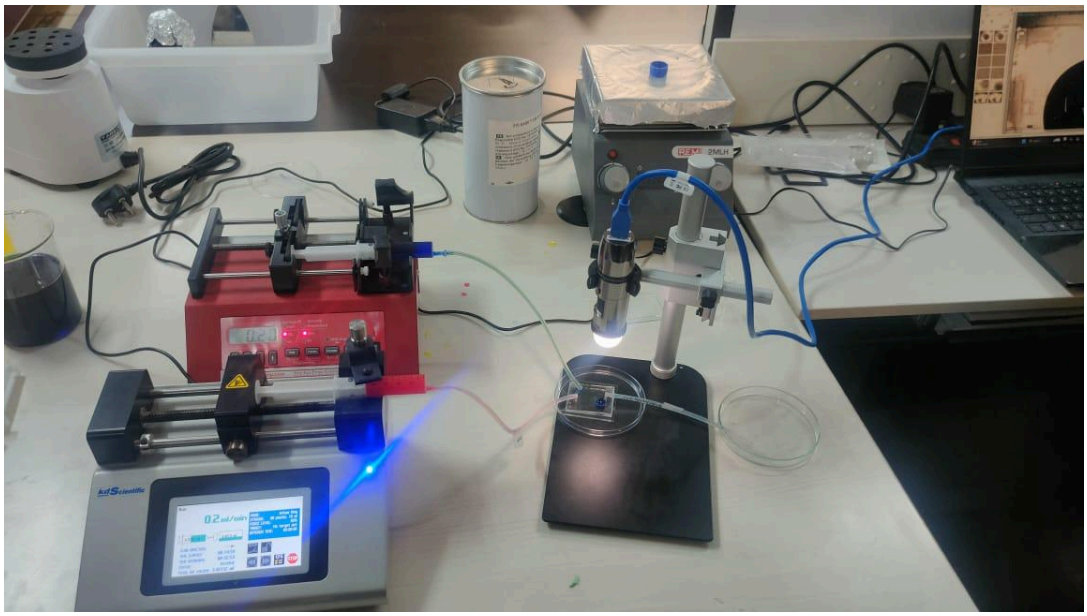

Fig 6: Experimental Setup

6. Conclusions

- A uniform gradient was achieved, ensuring proper mixing in the serpentine channels.
- Anomalous diffusion was observed, as the concentration gradient resembles with the concentration profile of anomalous diffusion.
- Higher flow rates resulted in a lower-slope gradient, confirming the impact of velocity on gradient formation.
- The numerical hydraulic resistance closely matched the analytical value, with a 6.09% error.
- The study emphasizes the role of flow control in optimizing microfluidic mixing for biomedical and chemical application

7. Future Scope

- **Geometric Optimization:** Further refinement of microchannel designs to enhance gradient uniformity, minimizing flow disturbances and dead zones.
- **Active Control Mechanisms:** Integration of external actuators or flow regulators to enable real-time adjustment of gradient profiles for dynamic applications.
- **Expanded Applications:** Potential applications in drug delivery systems, tissue engineering models, and chemical reaction kinetics studies.
- **Wastage Outlet Addition:** Introducing a dedicated waste outlet to prevent flow disturbances and allow clearer visualization of the gradient within the main observation region.
- **Electrokinetic and Thermal Effects:** Exploring electrokinetic flow control for enhanced mixing, along with thermal convection methods for fluids with different temperatures to modify diffusion characteristics dynamically.

References

[1]. Israelachvili, J. (2000) 'Generation of solution and surface gradients using microfluidic systems', *Langmuir*, 16(5), pp. 1891–1895.

[2]. Wang, X., Liu, Z. and Pang, Y. (2017) 'Concentration gradient generation methods based on microfluidic systems', *RSC Advances*, 7(44), pp. 27711–27745.