Designing of Microfluidic Concentration Generator Module for Self-Driving Fluid Mixing System

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1. Introduction

High-throughput self-driving laboratories can significantly accelerate material discovery. [1] For systems handling fluidic precursor solutions, precise and rapid concentration control is essential. Microfluidic devices are ideal for this purpose, offering high-throughput operation and precise fluid handling with minimal volume. To enable rapid customization for various mixing tasks, we propose a microfluidic concentration generator module design based on electric circuit analogy and 3D printing technology for integration into self-driving fluid mixing systems.

2. Channel Geometry Optimization

To mix fluids in microfluidic channels, we employ network-shaped channels based on the split-and-recombine (SAR) concept. With fixed network topology, we focus on optimizing channel geometry. For laminar, incompressible flow in microfluidic channels, electric circuit analogy enables efficient computation compared to high-cost computational fluid dynamics (CFD). [2, 3, 4] This analogy relates pressure difference to voltage, flow rate to current, and hydraulic resistance to electric resistance, allowing flow rate calculation using Kirchhoff's laws. We developed a modified Kirchhoff's current law (KCL) to compute concentrations. Since mass conservation of solutes holds at each node, the sum of incoming solute mass flow rates equals outgoing rates, enabling concentration calculation from flow rates. This rapid computation method enables channel length optimization to achieve target outlet concentrations. We employed Non-dominated Sorting Genetic Algorithm II (NSGA-II) [5] to solve this multi-objective, underdetermined optimization problem, minimizing both flow rate and concentration errors. This method generates arbitrary outlet concentrations as shown in Figure 1.

3. Application into Self-Driving Laboratories

Digital light processing (DLP)-based 3D printing enables rapid fabrication of optimized microfluidic concentration generator modules. [6, 7] Combined with our geometry optimization method, this allows easy customization for various fluid mixing tasks in self-driving laboratories. We designed a self-driving fluid mixing system (Figure 2) that mixes precursor solutions at various concentration ratios, dispenses mixed solutions onto substrates, and synthesizes materials by heating. For precise droplet dispensing, we developed a dynamic control algorithm and customized nozzle design. Droplet dispensing uses feedback control between the pressure controller and flow sensor, but suffers from time delay effects. We improved performance by smoothly adjusting PID controller parameters to compensate for delays. Our customized sharp, hydrophobic nozzle features a pinning dam to retain meniscus shape during dispensing, enabling precise droplet formation. These hardware and software improvements enable consistent, precise dispensing operation and full integration into autonomous laboratories for collecting control and synthesis data.

Acknowledgments

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4. Figures

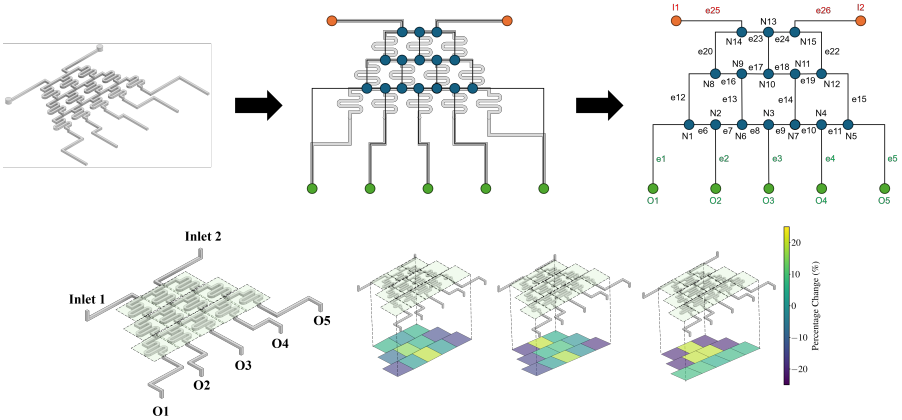

Fig. 1: Above: Transformation of a microfluidic channel network into a graph-based computational model. Below: The NSGA-II algorithm was used to generate optimised geometries for three different concentration targets. The heatmaps show the percentage length change of each segment compared to the reference design (see colour bar), demonstrating the geometric modifications needed to meet the targets.

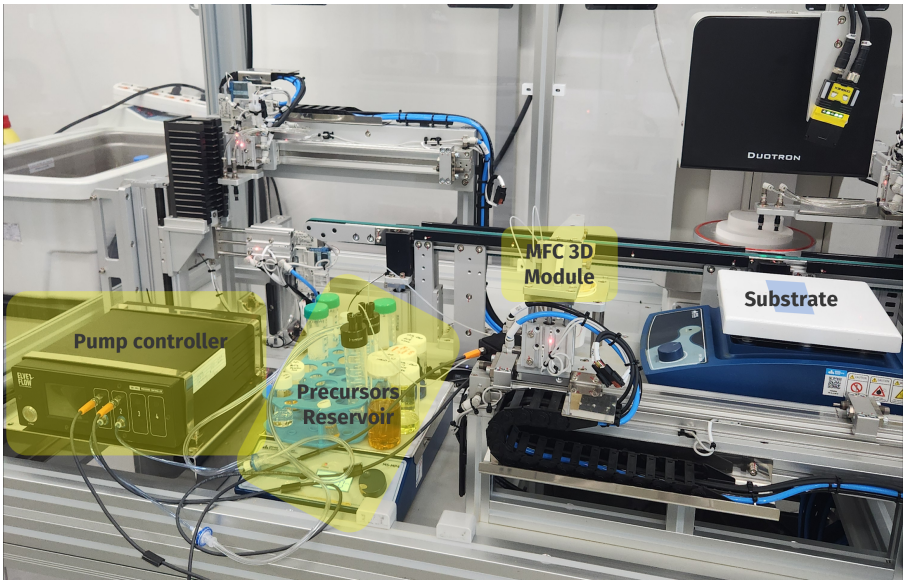

Fig. 2: Self-driving fluid mixing system integrated with the microfluidic concentration generator module.