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# CFD-based optimal design of manifold in plate-fin microdevices

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**Abstract**

Most microdevices are usually developed ad hoc, on the basis of engineers' experience—there is no systematic procedure for developing a microdevice. In this research, as the first step for the systematic design of microdevices, a design problem of a plate-fin microdevice was focused on, and characteristics of flow pattern inside plate-fin microdevices were investigated by using computational fluid dynamics (CFD). The simulation results show that the flow uniformity among branched microchannels depends largely on shapes of manifolds, length and location of fins, and inlet flow rate. A CFD-based optimization method is proposed for the design of plate-fin microdevices. With the proposed method, the optimal manifold shape that minimizes space time under the constraint on flow uniformity is automatically derived. The proposed method has a potential as an optimal design tool for various devices.


*Keywords:* Plate-fin microdevices; Manifold shape; Computational fluid dynamics (CFD); Automatic shape optimization; Robust design

## 1. Introduction

Microfabrication techniques progressed considerably in the field of electronics in the second half of the 20th century. Devices such as micropumps, microsensors, and microactuators are called micro electro mechanical systems (MEMS). Recently, MEMS have accelerated the advances in micro total analysis systems (μTAS) [1–6]. The key technologies of μTAS are microanalysis chips for chemical and biological applications such as DNA decoding equipment and on-site environmental monitoring systems. Miniaturization of chemical analytic devices reduces the amount of samples and cuts down the analysis time.

Since the mid 1990s, microfabrication has also opened new opportunities for chemical industries and micro chemical plants are expected to exceed the capabilities of conventional macroscopic plants [7–11]. Many types of microdevices, such as micro heat exchangers, micromixers, and microreactors, have been devised and manufactured. Those devices are important elements of micro chemical plants. The dominant characteristics of micro chemical plants are as follows: (a) the ratio of surface area to volume is very high, (b) the effective volume inside microdevices is very small, and (c) the field of flow is laminar. Analysis of chemical reactions and transport phenomena in microchannels or micro-spaces has been performed energetically [12–22]. In order to utilize microfabricated devices for chemical production, the technologies of design, operation, and control of micro chemical plants need to be systematized on the basis of the results of fundamental researches.

At present, most microdevices are designed and fabricated by trial and error—there is no systematic procedure for developing a microdevice. Therefore, it takes much time and effort to reach an optimal design. Unless this situation is improved, shortening of lead time is not expected. To achieve further breakthroughs in micro chemical plants' technologies, an approach to systematically design microdevices needs to be established.

In the field of MEMS, many efficient simulators have been developed to predict device performance in the last few years [23–26]. A lumped-parameter system is usually used in MEMS simulators to describe flow behavior, because a model should be simple in order to enhance design efficiency. But, when micro chemical plants are designed, microdevices need to be treated as distributed-parameter systems in order to analyze rigorously the characteristics of flow and heat transfer in them. Thus, MEMS simulators are inadequate for designing micro chemical plants.

In this study, to develop a new framework for the design of microdevices, characteristics of flow patterns inside plate-fin microdevices are investigated by using computational fluid dynamics (CFD). In addition to analysis of flow patterns, a CFD-based optimal design procedure is proposed.

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**Nomenclature**

| | |
|---|---|
| $A$ | manifold area |
| $f$ | dimensionless mass flow rate |
| $F$ | mass flow rate |
| $\bar{F}$ | average mass flow rate |
| $i$ | channel number |
| $L$ | length |
| $P$ | weighting factor |

*Greek letters*

| | |
|---|---|
| $\rho$ | density |
| $\eta$ | viscosity |

## 2. Effect of design parameters on flow uniformity

A plate-fin microdevice is one of the dominant devices used in a micro chemical plant. A plate-fin microdevice has multi-microchannels, which are parallel to each other and have the same shape and size. The representative plate-fin microdevice and the names of components are shown in Fig. 1. In order to execute a heterogeneous catalytic reaction inside a plate-fin microdevice, the surface of branched channels is often coated with catalysis. Since the ratio of surface area to volume is very high, the catalytic microreactors are expected to exceed conventional reactors in the yield and selectivity. However, the non-uniformity of flow residence time decreases the performance of catalytic microreactors. The non-uniformity is caused by laminar flow in microchannels and flow maldistribution among branched channels, and flow distribution is strongly affected by shape of device. The aim of this investigation is to design optimal plate-fin microdevices, which can distribute fluid equally into each channel.

In this work, Fluent® code is used to calculate three-dimensional flow distribution inside plate-fin microdevices. The finite-volume method with all the variables defined at the center of the control volumes is used in Fluent® to solve conservation equations for mass, momentum, and energy [27]. The equations are solved by using the SIMPLE algorithm. The Navier–Stokes equation with

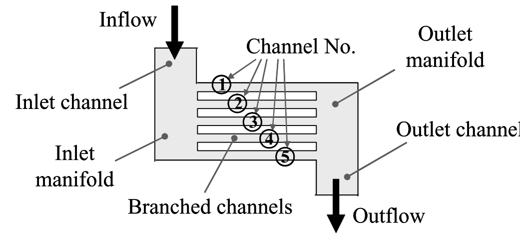


Fig. 1. A plate-fin microdevice (top view). Domains colored with light gray are filled with fluid.

non-slip boundary condition and negligible gravity is used to evaluate the flow characteristics. The Reynolds numbers for microchannels are usually considerably smaller than those for conventional macroscopic devices. Therefore, the microscopic flow through the channels can be assumed to be laminar.

### 2.1. Influence of branched channel length on flow distribution

Simulations of flow in microdevices with different channel length shown in Fig. 2 are carried out. Both depth and width of each branched channel are 100 μm. For every type of microdevice, the widths of the inlet channel, outlet channel, inlet manifold, and outlet manifold are the same, and each of them is equal to the sum of the widths of all five channels, 500 μm. Branched channel length is 1.5 mm (Type A-1), 4.5 mm (Type B-1), and 13.5 mm (Type D-1). Water ($\rho = 998.2\,\mathrm{kg/m^3}$, $\eta = 0.001\,\mathrm{kg/(m\,s)}$) is fed at a uniform velocity of 0.1, 0.5, or 1 m/s. At the outlet, the pressure is specified (atmospheric).

Fig. 2 shows the influence of branched channel length on flow distribution. Horizontal axis denotes channel number, and vertical axis denotes dimensionless mass flow rate, which is defined by

$$\bar{F} = \frac{1}{5}\sum_{i=1}^{5} F(i) \tag{1}$$

$$f(i) = \frac{F(i)}{\bar{F}} \tag{2}$$

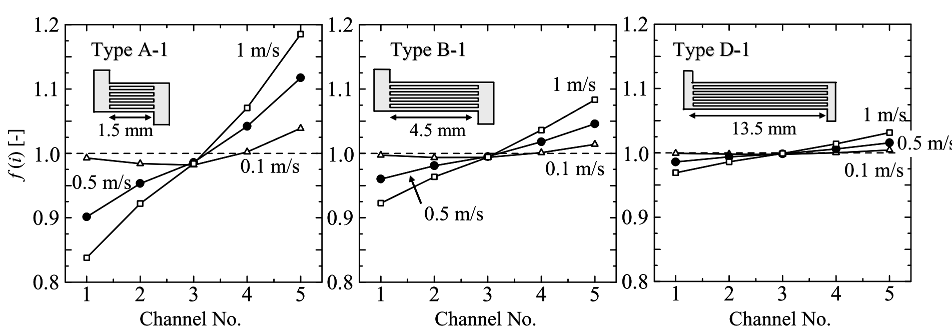


Fig. 2. Relation between channel length and flow distribution.

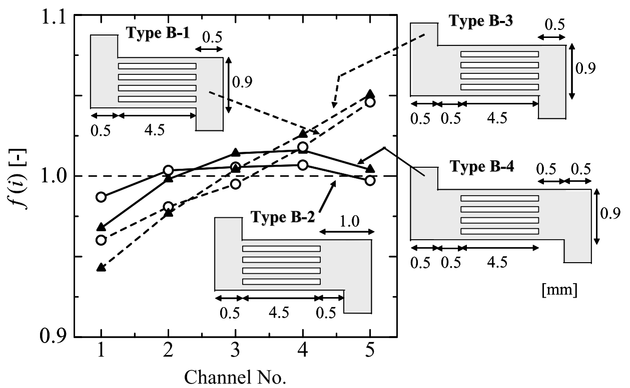


Fig. 3. Relation between manifold area and flow distribution.

As $f(i)$ ($i = 1, 2, \ldots, 5$) is closer to 1.0, flow uniformity becomes better. From the viewpoint of distributing fluid equally, Type D-1 is the best among Types A-1, B-1, and D-1. The longer channels enable fluid to be distributed equally into each channel, because pressure drop in channels becomes relatively larger than that in manifolds. These results suggest that the channel length has a considerable effect on the flow distribution.

### 2.2. Influence of manifold area on flow distribution

In this section, the influence of manifold area on the flow distribution is examined. Branched channel length is 4.5 mm, and manifold area is 500 μm × 900 μm or 1000 μm × 900 μm. Other design parameters except the length of branched channel and the size of manifolds are the same in Section 2.1. Fig. 3 shows the simulation results when water is fed at a uniform flow velocity of 0.5 m/s. The outlet manifold area of Type B-2 is twice as large as that of Type B-1. The flow distribution of Type B-2 is more uniform than that of Type B-1. Similarly, Type B-4 can realize more uniform flow distribution than Type B-3. These results demonstrate that the magnification of outlet manifold area makes the flow distribution uniform. Ehrfeld et al. [28] point out a similar result.

The effect of the manifold area on the flow distribution can be explained by investigating pressure distribution inside branched channels and the outlet manifold. Fig. 4 shows the contour plots of pressure distribution in Types B-1 and B-2. Acceleration of flow inside the outlet manifold reduces static pressure while increasing dynamic pressure. In Type B-1 with small outlet manifold, this phenomenon considerably affects pressure distribution inside branched channels, especially Nos. 4 and 5, and causes non-uniformity of flow in branched channels. The influence of flow acceleration can be reduced by expanding outlet manifold area. In fact, pressure distributions in each channel are almost the same in Type B-2 with large outlet manifold as shown in Fig. 4.

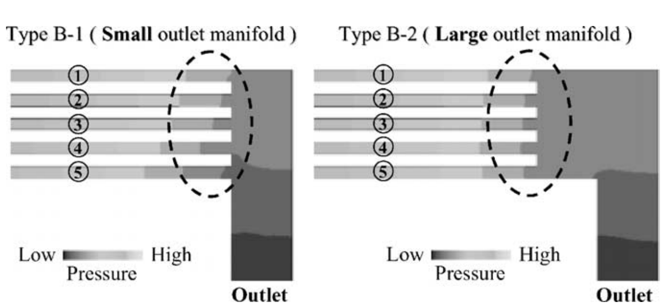


Fig. 4. Contour plots of pressure distribution (Types B-1 and B-2).

## 3. Optimization of manifold shape

Uniform flow distribution can be realized by extending outlet manifold area as shown in Section 2. However, the extension of the outlet manifold increases dead volume inside the microdevice, broadens residence time distribution, and lengthens space time. In general, these characteristics caused by extending outlet manifold area are undesirable because they decrease the efficiency of microdevices. Therefore, both size and shape of the manifold should be optimized to realize uniform flow distribution, desirable space time, and desirable residence time distribution simultaneously. In this section, the optimization problem of designing inlet and outlet manifolds is discussed. This design problem is very difficult to solve because an unlimited number of shapes should be tested in theory and microdevices cannot be treated as a lumped-parameter system. In the present work, the manifold shape is optimized by imposing constraints upon the shape and thereby reducing the degree of freedom.

### 3.1. Optimization of discretized shape

In the previous section, Type B-2 realizes the best flow distribution among four types. In this section, the space time minimization problem is discussed under the condition that a device realizes the same or more uniform flow distribution than Type B-2. Since the space time can be shortened by reducing manifold area, the optimization problem is formulated as follows:

$$\text{Minimize} \quad \text{Manifold area A} \tag{3}$$

$$\text{Subject to} \quad \sum_{i=1}^{5} \left| \frac{F(i) - \bar{F}}{\bar{F}} \right| \leq 0.05 \tag{4}$$

Fig. 5 shows the contour plot of velocity distribution in Type B-2. In this design, dead volume is formed around the corner of the manifold denoted by dotted circles. Dead volume lengthens space time and broadens residence time distribution. Therefore, we focused on the design of manifold having less dead volume. In this work, the corner of the manifold is trimmed away from the initial design Type B-2 in order to reduce the space time. The shape of the removed area is described to simplify the design problem. That is, a corner generated by connecting two black points at each manifold

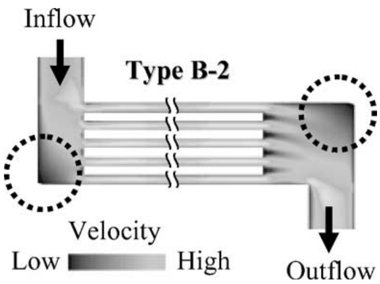


Fig. 5. Contour plot of velocity (Type B-2).

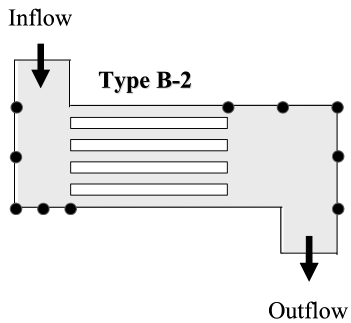


Fig. 6. Discrete model of manifolds.

shown in Fig. 6 is the removed manifold. By changing the combination of two points at each manifold, a total of 25 different shapes are generated. For all cases, flow patterns are simulated by CFD. As a result, more than half the cases do not satisfy the constraint of Eq. (4). Fig. 7 illustrates the best design (Type B-O) which achieves uniform flow distribution while satisfying constraint on flow uniformity. The manifold area of Type B-2 was cut by 25%. Fig. 8 shows flow distribution in Types B-2 and B-O.

### 3.2. Automatic shape optimization

It takes much time and effort to reach the optimal design if three-dimensional structures and meshes used in CFD simulations are manually generated for each device shape. For efficient design, an automatic shape optimization method needs to be developed.

In the optimization algorithm proposed in this section, the length of the borderlines defining the manifold shape is optimized as a continuous variable. Fig. 9 shows the flowchart

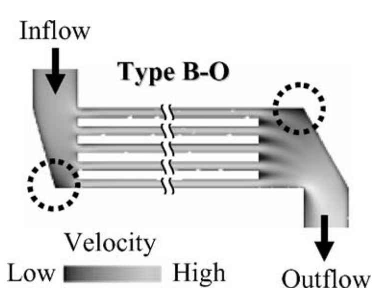


Fig. 7. Contour plot of velocity (Type B-O).

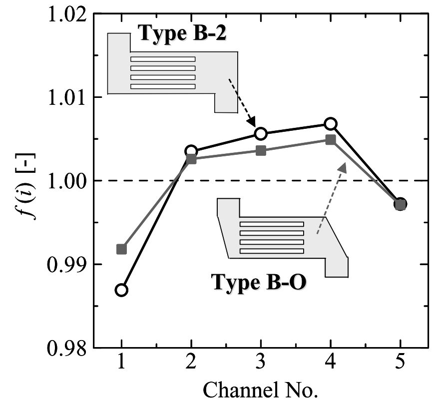


Fig. 8. Flow distribution (Types B-2 and B-O).

of the proposed algorithm to optimize the manifold shape. In the proposed method, the ranges of the optimization variables which define the shape of the device are given in advance. Then, the initial device shape is defined and meshes are generated manually. After a CFD simulation, the performance index is calculated. While the result is not optimal, the shape is updated and meshes are regenerated. The shape update and the mesh regeneration can be automatically executed by integrating the model and mesh generator (Gambit 2.1) with the CFD simulator (Fluent® 6.0) through Visual Basic 6.0. As a result, automatic shape optimization is realized in the present work.

As shown in Fig. 10, to simplify the problem, only the length of the upper line that forms the outlet manifold is treated as optimization variable. The Golden section search method [29] is used in the optimization algorithm. The objective function and constraint are Eqs. (5) and (6), respectively. The second term of the objective function indicates the degree of flow maldistribution. The weighting factor $P$ is determined by comparing the several optimization results

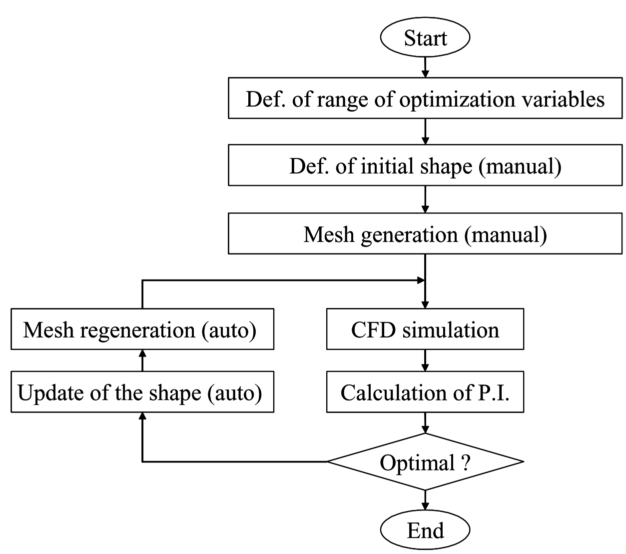


Fig. 9. Flowchart of shape optimization algorithm.

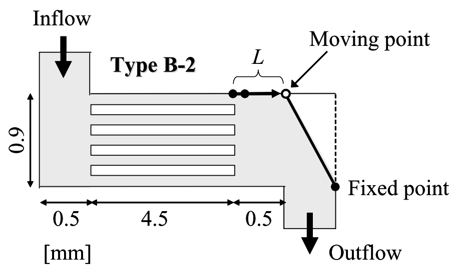


Fig. 10. Shape optimization of outlet manifold (Type B-2).

using different $P$ so that the desired balance between the area of manifold and the degree of flow maldistribution is achieved. It is difficult to select $P$ in advance. The sensitivity of the weighting factor $P$ to the optimal design depends on the characteristics of the design problem. In this problem, the optimal length is varied from 410 to 609 μm when $P$ changes from 5E−5 to 5E−4:

$$\text{Minimize} \quad A + P \times \sum_{i=1}^{5} \left| \frac{F(i) - \bar{F}}{\bar{F}} \right| \tag{5}$$

$$\text{Subject to} \quad 11\,\mu\text{m} \le L \le 1000\,\mu\text{m} \tag{6}$$

## 4. Results and discussion

### 4.1. Shape optimization

In the previous section, a shape optimization problem was formulated as one-dimensional optimization problem and was solved by using the proposed method. The results of the CFD-based shape optimization give a great deal of useful information on the design of microdevices to engineers. However, when the number of design variables increases, a huge amount of computational time is needed to obtain the optimal design. Another approach for the shape optimization is to use an aggregated model. Commenge et al. [30] have proposed an approximate model of a microreactor by using a network of equivalent rectangular ducts. This model makes it possible to rapidly calculate the velocity distribution inside the device. The dominant drawback is the difficulty of embedding the effect of the inertia of flow in the model. For example, the model should not be used when the direction of the inlet flow plays an important role. Therefore, the sequential use of two methods is a promising approach. First, the shape of the device is roughly determined by using an aggregated method. Then, precise calculation is executed by using the proposed CFD-based optimization method explained in the previous section.

### 4.2. Robust design of microdevice

The objective of using microdevices for chemical production is to achieve very high efficiency, which is difficult for conventional chemical plants to reach. To maximize the performance of microdevices, operating conditions must be tightly controlled. However, installing sensors and actuators in each microdevice is not practical because the number of instruments becomes excessively large. Therefore, it is crucial to design robust microdevices against disturbances and changes in operating conditions. In this section, the influence of fin location on flow distribution is examined for various inlet flow rates, and the fin location increasing the robustness of the microdevices is derived. A new microdevice, Type C, is created to equalize the flow pattern around the inlet of each branched channel and thereby to realize uniform flow distribution. Each fin in Type C is shifted in parallel as shown in Fig. 11. The space time of the fluid is the same for Types B-1 and C. CFD simulations were performed for three levels of inlet flow rates. The simulation results show that Type C is more robust than Type B-1 from the viewpoint of flow uniformity against changes in inlet flow rates. The maldistribution of fluid in Type B-1 seems to be caused by the influence of inertial force. Since the inertial force increases as the inlet flow rate becomes higher, flow uniformity is deteriorated at the high inlet flow rate. Type C can realize more uniform flow distribution than Type B-1 by shifting fins, equalizing flow pattern around inlet of each branched channel, and reducing the influence of inertia force. These results suggest that a robust micro chemical plant can be actualized without installing sensors and actuators by investing individual devices with robustness.

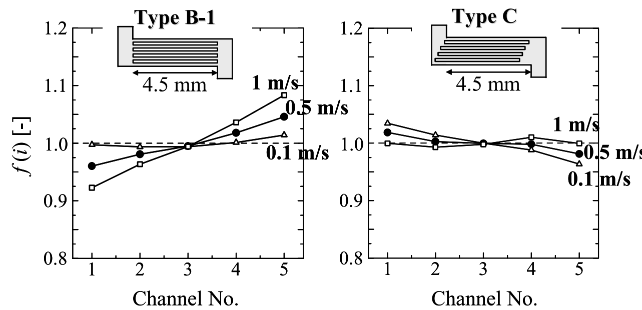


Fig. 11. Comparison between Type B-1 and Type C.

## 5. Conclusions

A plate-fin microdevice is one of the dominant devices used in a micro chemical plant. In this device, the flow uniformity in branched channels is very important for realizing the sharp residence time distribution. Flow distribution is strongly affected by shape of device; therefore, in this paper, effects of the design on the flow uniformity were discussed by using CFD simulation.

Simulation results show that longer branched channels enable fluid to be distributed equally into each channel. Also demonstrated is the fact that the magnification of the outlet manifold area makes the flow distribution uniform. However, the extension of the outlet manifold increases dead volume inside the microdevice, broadens residence time distribution, and lengthens space time.

In Section 3, the shape optimization problem to make space time small is solved under the constraint on flow uniformity. The result clarifies that a plate-fin microdevice with optimal manifold shape can achieve uniform flow distribution while realizing minimum space time. To derive the optimal shape automatically, a new optimization method was developed by integration of the model and mesh generator with the CFD simulator.

Furthermore, the effect of location of fins on flow uniformity was investigated for various inlet flow rates. The simulation results suggest the possibility of designing micro chemical plants with robustness.

Optimal micro chemical plant design requires the development of an efficient design method. The CFD-based optimization approach proposed in the present work can give rigorous results, but it requires considerable computational time. To accelerate the design, a sequential design method would be useful. That is, a simplified model is used at initial design stage to roughly select good device shape, and then a rigorous CFD simulation is performed to determine an optimal design. At this stage of the development, it is not clear what kind of simplification of a device model is suitable for efficient design and is consistent with a rigorous model used in CFD simulation. Further efforts are necessary in this research area.

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