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# A method for the identification of multiple blocked locations in a microreactor without a combinatorial explosion of CFD simulations for database construction

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## Abstract

Microreactors with parallelized microchannels are widely used in chemical industries because a single microchannel processes only a small amount of raw material. Any blockage in parallelized microchannels causes poor uniformity of the residence time distribution among the microchannels, which leads to degrade product quality. To address this issue, we developed a method for the identification of multiple blocked locations. The method identifies blockage locations by comparing measured pressure distribution data with pressure distribution data that is calculated by computational fluid dynamic (CFD) simulation when blockage occurs. For this research, we extended the method to apply to cases in which there are three or more blocked microchannels without incurring any combinatorial explosion of CFD simulations for the database construction. The proposed method identifies multiple blocked locations using only pressure distribution data obtained when each single microchannel in a microreactor is blocked. The results of CFD simulations showed that the method accurately identified three blocked locations by using fewer pressure sensors than there were microchannels.

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*Keywords:* Microreactor; Diagnosis; Blockage; Computational fluid dynamics; Database

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## 1. Introduction

A microreactor is a new type of production technology for specialty chemicals that are difficult to produce with conventional reactors [1-2]. Industrial-scale microreactors require a large number of parallelized microchannels because each one provides only a small amount of product.

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Nomenclature		
$BD$	blockage degree	[%]
$f$	flow rate	[m <sup>3</sup> /s]
$I$	set of microchannel	[-]
$i$	channel number	[-]
$l$	length	[m]
$n$	number	[-]
$P$	pressure data vector	[Pa]
$p$	pressure	[Pa]
$R$	correlation coefficient	[-]
$S$	set of sensor locations	[-]
$s$	sensor location	[-]
$v$	inlet velocity	[m/s]
$w$	width	[m]
$z$	depth	[m]
$\mu$	viscosity	[Pa·s]
<subscripts>		
B	blocked condition	
bot	bottom	
C	channel	
F	fin (Channel wall)	
M	manifold	
N	normal condition	
O	outlet	
top	top	

Microchannels are prone to blockage due to side reactions or contamination from raw materials when they are operated for a long period. Blockage in microchannels causes poor uniformity in the residence time distribution among them, leading to degraded product quality. Blockage in the microchannels of microreactors is a serious problem that limits their practicality. It is therefore essential to detect and identify blockage locations to ensure more effective and stable microreactor operation.

Kano *et al.* [3] proposed data-based and model-based blockage diagnosis methods using temperature sensors that identify a blockage location in stacked microchemical processes. The data-based method compares the ratios of temperature differences between normal and abnormal operating conditions at one sensor to those at the other sensor. The simulation results showed that this method could diagnose the blockage location successfully. However, it might not work if the blockage does not affect the temperature in a microreactor due to its high surface/volume ratio.

Tanaka *et al.* [6] developed a blockage detection and diagnosis system for parallelized microreactors with split-and-recombine-type flow distributors. This system can isolate a blocked microreactor with a small number of flow sensors. Yamamoto *et al.* [7] proposed a method that uses pressure sensors instead of temperature sensors, in which the blockage location is identified by comparing measured pressure distribution data with prepared pressure distribution data calculated by computational fluid dynamic (CFD) simulation when a blockage occurs. Simulation results showed that these methods could diagnose a single blockage location using

fewer pressure sensors than microchannels. However, if this method is applied to an abnormal situation in which blockage occurs at multiple channels, a large amount of pressure distribution data for all combinations of multiple blocked channels under varying degrees of blockage is necessary for construction of a database, which causes a combinatorial explosion of CFD simulations.

To prevent this problem of CFD simulations, we previously proposed a data-based blockage diagnosis method that can identify blockages in two microchannels with a small database [4-5]. The method identifies blocked locations from just pressure distribution data when a single channel is blocked for a single blockage degree. The total number of CFD simulations to construct the database is considerably smaller than that with the previous method. However, the method cannot be applied to an abnormal situation in which blockage occurs at any number of microchannels. For this research, we extended the method to apply to cases in which there are three or more blocked microchannels without incurring any combinatorial explosion of CFD simulations for database construction. CFD simulation was used in this study to generate the validation data for our method in the case studies.

## 2. Microreactor

A microreactor generally consists of three parts: an inlet manifold for flow distribution, parallelized microchannels for the reaction, and an outlet manifold for mixing. Figure 1 shows the structure of the point symmetrical microreactor used for the study. Industrial-scale production using a microreactor requires a high number of parallelized microchannels because each one provides only a small amount of product. Blockage in the microchannel causes poor uniformity in the residence time distribution between them, which may worsen product quality.

The blockage degree  $BD_i$  of microchannel  $i \in I$  in a microreactor is defined by using Eq. (1), where  $f_{B,i}$  and  $f_{N,i}$  are the flow rates of microchannel  $i$  with and without blockage, respectively [3]. Here,  $I$  is the set of microchannel numbers.

$$BD_i = \left( 1 - \frac{f_{B,i}}{f_{N,i}} \right) \times 100 \text{ [%]} \quad (1)$$

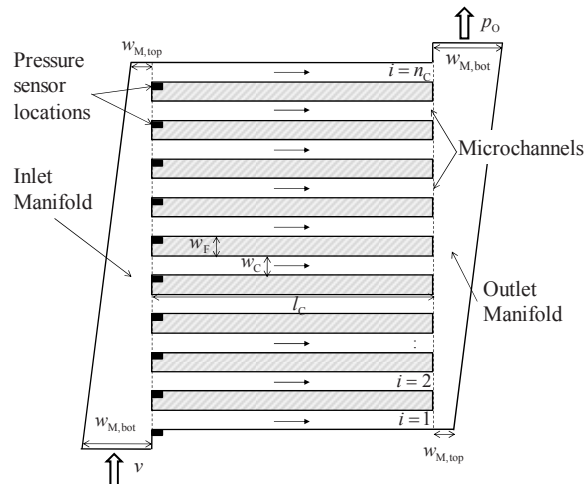


Fig. 1. Structure of microreactor

### 3. Diagnosis method of multiple blockage locations

The pressure drop distribution in a microreactor changes when a blockage occurs. The pressure distribution has certain patterns with regard to blockage locations. Therefore, the locations can be identified by comparing the measured pressure distribution data with pressure distribution data prepared before the blockages occurred.

To construct a database for identifying multiple blocked channels, it is necessary to calculate a large amount of pressure distribution data for every combination of multiple channels under various degrees of blockage, which is a very time-consuming process.

#### 3.1. Database construction

To prevent a combinatorial explosion of CFD simulations, we propose a simple method for identifying multiple blockage locations from just the prepared pressure distribution data when a single channel is blocked. The procedure for building the database is as follows.

- (1) Measure pressure distribution data vector  $\tilde{P}_N$  consisting of measured pressure  $\tilde{p}_{N,s}$  ( $s \in S$ ) without any blockage. Here,  $\tilde{p}_{N,s}$  denotes the pressure data measured at sensor location  $s$  and  $S$  is the set of sensor locations.
- (2) Calculate pressure distribution data vector  $\hat{P}_{B,i}$  ( $i \in I$ ) consisting of  $\hat{p}_{B,i,s}$  ( $i \in I, s \in S$ ) by CFD simulation. Here,  $\hat{p}_{B,i,s}$  denotes the calculated pressure data at sensor location  $s$  under a certain blockage degree in channel  $i$ .
- (3) Calculate pressure difference data vector  $\Delta\hat{P}_{B,i}$  by using Eq. (2).

$$\Delta\hat{P}_{B,i} = \hat{P}_{B,i} - \tilde{P}_N \quad (i \in I) \quad (2)$$

In this method, the total number of CFD simulations for database construction is always equal to that of microchannels and does not change according to number of blocked microchannels.

#### 3.2. Identification method of multiple blocked locations

The  $n_B$  blocked microchannels are identified through the following procedures.

- (1) Obtain actual pressure data vector  $\tilde{P}_B$  consisting of  $\tilde{p}_{B,s}$  ( $s \in S$ ).
- (2) Calculate actual pressure difference data vector  $\Delta\tilde{P}$  by Eq. (3).

$$\Delta\tilde{P} = \tilde{P}_B - \tilde{P}_N \quad (3)$$

- (3) Calculate the orthogonal projection vector  $\Delta\bar{P}$  of  $\Delta\tilde{P}$  to the projection plane spanned by vectors  $\Delta\hat{P}_{B,i_1}, \Delta\hat{P}_{B,i_2}, \dots, \Delta\hat{P}_{B,i_{n_B}}$  ( $i_1, i_2, \dots, i_{n_B} \in I$ ) by using Eqs. (4) and (5), where  $\langle \cdot, \cdot \rangle$  denotes the inner product,  $\|\cdot\|$  denotes the 2-norm, and  $i_1, i_2, \dots, i_{n_B}$  are all combinations of  $n_B$  microchannels.

$$\Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}} = \sum_{i=i_1, i_2, \dots, i_{n_B}} \alpha_i \Delta\hat{P}_{B, i} \quad (i_1, i_2, \dots, i_{n_B} \in I) \quad (4)$$

$$\begin{bmatrix} \alpha_{i_1} \\ \alpha_{i_2} \\ \vdots \\ \alpha_{i_{n_B}} \end{bmatrix} = \begin{bmatrix} \|\Delta\hat{P}_{B, i_1}\|^2 & \langle \Delta\hat{P}_{B, i_1}, \Delta\hat{P}_{B, i_2} \rangle & \cdots & \langle \Delta\hat{P}_{B, i_1}, \Delta\hat{P}_{B, i_{n_B}} \rangle \\ \langle \Delta\hat{P}_{B, i_1}, \Delta\hat{P}_{B, i_2} \rangle & \|\Delta\hat{P}_{B, i_2}\|^2 & & \langle \Delta\hat{P}_{B, i_2}, \Delta\hat{P}_{B, i_{n_B}} \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle \Delta\hat{P}_{B, i_1}, \Delta\hat{P}_{B, i_{n_B}} \rangle & \langle \Delta\hat{P}_{B, i_2}, \Delta\hat{P}_{B, i_{n_B}} \rangle & \cdots & \|\Delta\hat{P}_{B, i_{n_B}}\|^2 \end{bmatrix}^{-1} \begin{bmatrix} \langle \Delta\tilde{P}, \Delta\hat{P}_{B, i_1} \rangle \\ \langle \Delta\tilde{P}, \Delta\hat{P}_{B, i_2} \rangle \\ \vdots \\ \langle \Delta\tilde{P}, \Delta\hat{P}_{B, i_{n_B}} \rangle \end{bmatrix} \quad (5)$$

- (4) Calculate the correlation coefficient  $R_{i_1, i_2, \dots, i_{n_B}}$  between  $\Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}}$  and  $\Delta\tilde{P}$ . This coefficient is defined by

$$R_{i_1, i_2, \dots, i_{n_B}} = \frac{(\Delta\tilde{P} - \Delta\tilde{P}^m)^T (\Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}} - \Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}}^m)}{\|\Delta\tilde{P} - \Delta\tilde{P}^m\| \|\Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}} - \Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}}^m\|} \quad (i_1, i_2, \dots, i_{n_B} \in I) \quad (6)$$

where all elements of  $\Delta\tilde{P}^m$  and  $\Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}}^m$  are the means of all elements of  $\Delta\tilde{P}$  and  $\Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}}$ , respectively. The superscript T denotes the transpose.

- (5) Identify blocked microchannels  $i_1^*, i_2^*, \dots, i_{n_B}^*$  by using Eq. (7), whose microchannels have the highest correlation between  $\Delta\tilde{P}$  and  $\Delta\bar{P}_{i_1, i_2, \dots, i_{n_B}}$ .

$$(i_1^*, i_2^*, \dots, i_{n_B}^*) = \arg \max_{i_1^*, i_2^*, \dots, i_{n_B}^* \in I} R_{i_1, i_2, \dots, i_{n_B}} \quad (7)$$

#### 4. Case studies

In this section, we discuss the effectiveness of the proposed method as assessed through two case studies. Fluent<sup>TM</sup> ver. 6.1 (ANSYS Japan Co.) was used to generate validation data and a data set for the database.

##### 4.1. Objective microreactor

The proposed method was applied to the blockage diagnosis problems of a microreactor with 10 microchannels, which is shown in Figure 1. Pressure sensors were set up at the inlet of the microchannels  $i \in S$ . The measurement accuracy of the pressure sensors was assumed to be 10 Pa, which was determined in accordance with the best measurement accuracy of commercial micro electro mechanical systems (MEMS) sensors. The geometric parameters and the operating conditions of the microreactor are summarized in Table 1. The temperature and feed flow rate of the microreactor was controlled and kept constant.

Table 1. Geometric parameters and operation conditions of microreactor

Name	Parameters	Value	Unit
Number of channels	$n_C$	10	-
Channel width	$w_C$	100	$\mu\text{m}$
Channel depth	$z_C$	100	$\mu\text{m}$
Channel length	$l_C$	20	mm
Width of fin	$w_F$	284	$\mu\text{m}$
Viscosity	$\mu$	0.1	$\text{Pa}\cdot\text{s}$
Width of manifold	$w_{M,\text{top}}$	1.0	mm
	$w_{M,\text{bot}}$	5.0	mm
Inlet velocity	$v$	0.01	m/s
Outlet pressure	$p_O$	101.3	kPa

Two blockage diagnosis problems, Case 1 and Case 2, were considered to assess the proposed method's effectiveness, where four pressure sensor configurations (Conf. A–D) were implemented. In case studies, one of the blocked channels,  $i_1$ , was fixed at one or two to reduce the total number of CFD simulations.

$$\begin{aligned} \text{Conf. A:} & \quad n_S = 10, \quad S = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10\} \\ \text{Conf. B:} & \quad n_S = 6, \quad S = \{1, 3, 5, 6, 8, 10\} \\ \text{Conf. C:} & \quad n_S = 5, \quad S = \{1, 3, 5, 7, 9\} \\ \text{Conf. D:} & \quad n_S = 4, \quad S = \{1, 4, 7, 10\} \end{aligned}$$

$$\text{Case 1: } BD_{i_1} = 15\%, \quad BD_{i_2} = 35\%, \quad BD_{i_3} = 35\% \quad (i_1 = 1, i_2, i_3 \in I, i_1 < i_2 < i_3)$$

$$\text{Case 2: } BD_{i_1} = 15\%, \quad BD_{i_2} = 35\%, \quad BD_{i_3} = 35\% \quad (i_1 = 2, i_2, i_3 \in I, i_1 < i_2 < i_3)$$

#### 4.2. Diagnosis results

Ten CFD simulations were executed to obtain pressure distribution data under 50% blockage in each microchannel. The simulation results were then used as a data set in a database. Then, sixty-four CFD simulations were executed to obtain a validation data set for thirty-six combinations of three blocked channels for Case 1 and twenty-eight combinations of three blocked channels for Case 2.

Simulation results for Cases 1 and 2 are respectively summarized in Tables 2 and 3, in which the combinations of identified numbers of three blocked channels are shown. Several misdiagnoses occurred, which are denoted with underlines in the tables. Table 4 lists the percentages of correct diagnoses for sensor configurations A–D. The method perfectly identified the three blockage locations for both Cases 1 and 2 when using ten pressure sensors (Conf. A). The performance of the proposed method deteriorated when the number of pressure sensors decreased. However, when using six or five sensors (Conf. B and Conf. C), the method still correctly identified the three blocked microchannels in most cases: 100 and 94.4% for Case 1 and 96.4 and 89.3% Case 2. The average correct diagnosis percentage was 36.1% for Case 1 and 21.4% for Case 2 when the number of sensors was four. This is because too small a number of sensors make it impossible to distinguish the changes in patterns of pressure distribution with regard to blockage locations.

The average correct diagnosis percentages using six sensors (Conf. B) was 94.5% when the number of blocked channels are two [4]. These results demonstrate that a small database with pressure distribution data for the blockage in a single microchannel can correctly identify multiple blockage locations in a microreactor when the number of pressure sensors is more than half that of microchannels.

Table 2. Diagnosis results of case 1

No.	Blocked channels	Sensor configurations ( $n_s$ )			
		A(10)	B(6)	C(5)	D(4)
1	1, 2, 3	1, 2, 3	1, 2, 3	1, 2, 3	<u>2, 3, 8</u>
2	1, 2, 4	1, 2, 4	1, 2, 4	1, 2, 4	<u>1, 4, 5</u>
3	1, 2, 5	1, 2, 5	1, 2, 5	1, 2, 5	<u>1, 2, 7</u>
4	1, 2, 6	1, 2, 6	1, 2, 6	1, 2, 6	<u>1, 5, 6</u>
5	1, 2, 7	1, 2, 7	1, 2, 7	1, 2, 7	1, 2, 7
6	1, 2, 8	1, 2, 8	1, 2, 8	1, 2, 8	<u>2, 3, 8</u>
7	1, 2, 9	1, 2, 9	1, 2, 9	1, 2, 9	<u>2, 3, 9</u>
8	1, 2, 10	1, 2, 10	1, 2, 10	1, 2, 10	1, 2, 10
9	1, 3, 4	1, 3, 4	1, 3, 4	1, 3, 4	<u>2, 4, 8</u>
10	1, 3, 5	1, 3, 5	1, 3, 5	1, 3, 5	<u>2, 5, 8</u>
11	1, 3, 6	1, 3, 6	1, 3, 6	<u>2, 3, 6</u>	<u>1, 5, 7</u>
12	1, 3, 7	1, 3, 7	1, 3, 7	1, 3, 7	<u>1, 9, 10</u>
13	1, 3, 8	1, 3, 8	1, 3, 8	1, 3, 8	<u>2, 6, 8</u>
14	1, 3, 9	1, 3, 9	1, 3, 9	1, 3, 9	<u>2, 9, 10</u>
15	1, 3, 10	1, 3, 10	1, 3, 10	1, 3, 10	<u>1, 3, 10</u>
16	1, 4, 5	1, 4, 5	1, 4, 5	1, 4, 5	<u>2, 3, 8</u>
17	1, 4, 6	1, 4, 6	1, 4, 6	1, 4, 6	<u>1, 3, 10</u>
18	1, 4, 7	1, 4, 7	1, 4, 7	1, 4, 7	1, 4, 7
19	1, 4, 8	1, 4, 8	1, 4, 8	1, 4, 8	<u>6, 7, 10</u>
20	1, 4, 9	1, 4, 9	1, 4, 9	1, 4, 9	<u>6, 7, 9</u>
21	1, 4, 10	1, 4, 10	1, 4, 10	1, 4, 10	1, 4, 10
22	1, 5, 6	1, 5, 6	1, 5, 6	<u>3, 4, 8</u>	<u>2, 6, 8</u>
23	1, 5, 7	1, 5, 7	1, 5, 7	1, 5, 7	1, 5, 7
24	1, 5, 8	1, 5, 8	1, 5, 8	1, 5, 8	<u>2, 9, 10</u>
25	1, 5, 9	1, 5, 9	1, 5, 9	1, 5, 9	<u>2, 6, 9</u>
26	1, 5, 10	1, 5, 10	1, 5, 10	1, 5, 10	<u>2, 8, 9</u>
27	1, 6, 7	1, 6, 7	1, 6, 7	1, 6, 7	<u>3, 4, 7</u>
28	1, 6, 8	1, 6, 8	1, 6, 8	1, 6, 8	1, 6, 8
29	1, 6, 9	1, 6, 9	1, 6, 9	1, 6, 9	1, 6, 9
30	1, 6, 10	1, 6, 10	1, 6, 10	1, 6, 10	1, 6, 10
31	1, 7, 8	1, 7, 8	1, 7, 8	1, 7, 8	1, 7, 8
32	1, 7, 9	1, 7, 9	1, 7, 9	1, 7, 9	<u>3, 4, 5</u>
33	1, 7, 10	1, 7, 10	1, 7, 10	1, 7, 10	<u>1, 6, 8</u>
34	1, 8, 9	1, 8, 9	1, 8, 9	1, 8, 9	1, 8, 9
35	1, 8, 10	1, 8, 10	1, 8, 10	1, 8, 10	1, 8, 10
36	1, 9, 10	1, 9, 10	1, 9, 10	1, 9, 10	1, 9, 10

Table 3. Diagnosis results of case 2

No.	Blocked channels	Sensor configurations ( $n_s$ )			
		A(10)	B(6)	C(5)	D(4)
1	2, 3, 4	2, 3, 4	<u>1, 3, 4</u>	2, 3, 4	<u>2, 4, 5</u>
2	2, 3, 5	2, 3, 5	2, 3, 5	2, 3, 5	<u>2, 4, 5</u>
3	2, 3, 6	2, 3, 6	2, 3, 6	2, 3, 6	<u>1, 3, 6</u>
4	2, 3, 7	2, 3, 7	2, 3, 7	2, 3, 7	2, 3, 7
5	2, 3, 8	2, 3, 8	2, 3, 8	2, 3, 8	<u>3, 4, 8</u>
6	2, 3, 9	2, 3, 9	2, 3, 9	2, 3, 9	2, 3, 9
7	2, 3, 10	2, 3, 10	2, 3, 10	2, 3, 10	<u>1, 3, 7</u>
8	2, 4, 5	2, 4, 5	2, 4, 5	2, 4, 5	<u>3, 4, 6</u>
9	2, 4, 6	2, 4, 6	2, 4, 6	2, 4, 6	<u>3, 4, 6</u>
10	2, 4, 7	2, 4, 7	2, 4, 7	2, 4, 7	2, 4, 7
11	2, 4, 8	2, 4, 8	2, 4, 8	2, 4, 8	<u>4, 6, 7</u>
12	2, 4, 9	2, 4, 9	2, 4, 9	2, 4, 9	<u>2, 3, 10</u>
13	2, 4, 10	2, 4, 10	2, 4, 10	2, 4, 10	2, 4, 10
14	2, 5, 6	2, 5, 6	2, 5, 6	2, 5, 6	<u>1, 3, 5</u>
15	2, 5, 7	2, 5, 7	2, 5, 7	2, 5, 7	<u>4, 6, 9</u>
16	2, 5, 8	2, 5, 8	2, 5, 8	2, 5, 8	<u>1, 2, 4</u>
17	2, 5, 9	2, 5, 9	2, 5, 9	2, 5, 9	<u>7, 9, 10</u>
18	2, 5, 10	2, 5, 10	2, 5, 10	2, 5, 10	2, 5, 10
19	2, 6, 7	2, 6, 7	2, 6, 7	2, 6, 7	<u>6, 9, 10</u>
20	2, 6, 8	2, 6, 8	2, 6, 8	2, 6, 8	<u>4, 6, 7</u>
21	2, 6, 9	2, 6, 9	2, 6, 9	2, 6, 9	<u>4, 5, 10</u>
22	2, 6, 10	2, 6, 10	2, 6, 10	2, 6, 10	<u>4, 7, 8</u>
23	2, 7, 8	2, 7, 8	2, 7, 8	2, 7, 8	<u>4, 6, 7</u>
24	2, 7, 9	2, 7, 9	2, 7, 9	2, 7, 9	<u>6, 9, 10</u>
25	2, 7, 10	2, 7, 10	2, 7, 10	2, 7, 10	2, 7, 10
26	2, 8, 9	2, 8, 9	2, 8, 9	<u>2, 5, 10</u>	<u>1, 7, 8</u>
27	2, 8, 10	2, 8, 10	2, 8, 10	<u>2, 8, 9</u>	<u>2, 6, 9</u>
28	2, 9, 10	2, 9, 10	2, 9, 10	<u>2, 8, 9</u>	<u>1, 8, 9</u>

Table 4. Diagnosis results of proposed method

Conf. ( $n_s$ )	A(10)	B(6)	C(5)	D(4)
Case 1	100 %	100 %	94.4 %	36.1 %
Case 2	100 %	96.4 %	89.3 %	21.4 %

## 5. Conclusion

A data-based identification method that can identify blockages in multiple microchannels was proposed. To prevent a combinatorial explosion of CFD simulations for database construction, the proposed method identifies blocked locations by using only pressure distribution data when a single channel is blocked. The



results of CFD simulations showed that the method could accurately identify three blockage locations using fewer pressure sensors than there were microchannels. We focused on a case in which three microchannels were blocked, but our method can be easily applied to cases in which there are four or more blocked microchannels without incurring any combinatorial explosion of CFD simulations for database construction. In the proposed method, it is assumed that the number of blocked channels is known when identifying the locations of blocked channels. I intend to work on developing a method to estimate the number of blocked channels in my future research.

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