11th World Congress on Structural and Multidisciplinary Optimization
7th - 12th, June 2015, Sydney Australia

Level Set-Based Topology Optimization Using the Lattice Boltzmann Method Considering Two-Phase Fluid Flows

Kentaro Yaji[1], Takayuki Yamada[2], Masato Yoshino[3], Toshiro Matsumoto[4], Kazuhiro Izui[5], Shinji Nishiwaki[6]

[1] Kyoto University, Kyoto, Japan, yaji.kentarou.74v@kyoto-u.ac.jp
[2] Kyoto University, Kyoto, Japan, takayuki@me.kyoto-u.ac.jp
[3] Shinshu University, Nagano, Japan, masato@shinshu-u.ac.jp
[4] Nagoya University, Nagoya, Japan, t.matsumoto@nuem.nagoya-u.ac.jp
[5] Kyoto University, Kyoto, Japan, izui@me.kyoto-u.ac.jp
[6] Kyoto University, Kyoto, Japan, shinji@prec.kyoto-u.ac.jp

1. Abstract
This paper presents a topology optimization method using the lattice Boltzmann method for the design of a flow channel considering two-phase fluid flows. This approach enables the design of fluidic devices such as two-phase microchannels that achieve a desired flow with maximal performances such as mixing and reaction, and extraction efficiencies. The optimization problems are formulated using the continuous Boltzmann equation, and the design sensitivities are derived based on the adjoint lattice Boltzmann method. In the adjoint lattice Boltzmann method, based on a novel discretization strategy similar to that of the lattice Boltzmann method, the adjoint equations can be implemented as simple time evolution equations. Based on the above formulations, we construct a topology optimization method incorporating level set boundary expressions for the design of a two-phase microchannel that aims to maximize extraction efficiency while minimizing the pressure drop. A numerical example is provided to confirm the utility of the proposed method.
2. Keywords: Topology Optimization, Lattice Boltzmann Method, Two-Phase Flow, Level Set Method

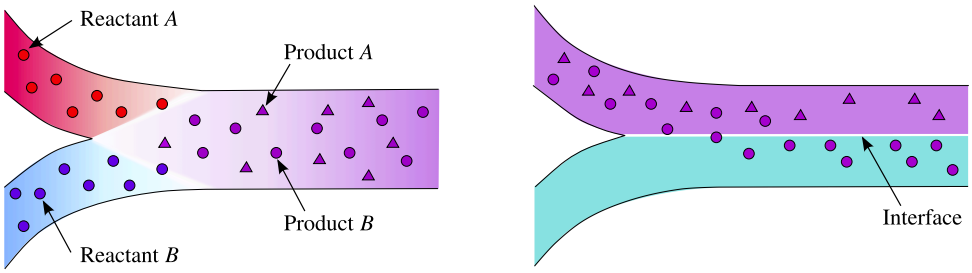
3. Introduction
The aim of this research is to construct a topology optimization method for the design of a flow channel considering two-phase fluid flows. Using this approach, fluidic devices such as two-phase microchannels can be designed so that they achieve a desired flow and accomplish maximal mixing and reaction, or extraction efficiencies.

These performances strongly depend on the design of the channel configuration, so that each process, such as mixing, reaction, or extraction, is finished as quickly as possible (Fig. 1). In addition, to prevent damage to the microchannels, minimizing the pressure drop in the microchannel system is an important factor. Thus, to meet the most important design requirements of a two-phase microchannel, the maximization of the above efficiencies and the minimization of the pressure drop must be simultaneously considered. Designer intuition alone, however, seldom yields an optimal channel configuration that sufficiently satisfies these requirements.

To overcome this problem, topology optimization [1] is a particularly powerful approach for obtaining useful designs for the channel configuration of the devices under consideration here. The basic concept of topology optimization is the introduction of an extended design domain, the so-called fixed design domain, and the replacement of the optimization problem with a material distribution problem, using the characteristic function. Borravall and Petersson [2] pioneered a topology optimization method for a dissipation energy minimization problem under Stokes flow, in which the material distribution in the fixed design domain is represented as consisting of either fluid or solid domains.

Based on this methodology, Okkels and Bruus [3] proposed a topology optimization method for the design of a micro reactor in which the reaction effect is mathematically modeled, and the aim was to achieve maximal reaction efficiency in the microchannel system given a uniform concentration of reactants. Andreasen et al. [4] proposed a topology optimization method for the design of a micro mixer in which maximization of mixing performance was the aim. And Makhija et al. [5] applied the lattice Boltzmann method (LBM) [6] in mixing performance maximization problem and investigated the relationship between the mixing performance and the pressure drop.

The basic idea of the above optimization methodologies for multi-component fluid flows is the introduction of concentration, governed by a convective-diffusion equation, into the formulation of the optimization problem. That is, since the fluid flow is not affected by concentration (one-way coupling), the above research cannot treat fluid flows of immiscible liquids in which the interface effect between the two phases must be considered. In particular, since the extraction process strongly depends on the difference between molecular diffusive coefficients



(a) Mixing & Reaction (b) Extraction

Figure 1: Schematic diagram of typical experiments in microchannel device.

in two-phase fluid flows [7], the conventional approach must be extended so that flows can be treated in extraction efficiency maximization problems.

Here, we construct a new topology optimization method for an extraction efficiency maximization problem, in which two-phase fluid flows are analyzed based on the two-phase LBM proposed by Inamuro et al. [8]. Since special treatments for tracking an interface are unnecessary in this method, the LBM is suitable for the computation of multi-phase fluid flows. In addition, since the LBM is an explicit scheme based on a simple time evolution equation, the adjoint equation can be formulated with this equation that is discretized using the LBM [9]. Previously, we investigated the applicability of this *adjoint lattice Boltzmann method* to topology optimization problems, and verified that this approach enables the design sensitivity to be quickly obtained at each optimization step [10].

In the following section, the basic concept of the two-phase LBM is discussed and the topology optimization problem is formulated for the extraction efficiency maximization problem. The numerical implementations and optimization algorithms are then explained and, finally, we provide a numerical example to validate the utility of the proposed method.

4. Formulation

4.1. Two-Phase Lattice Boltzmann Method

We now discuss the concept of the two-phase LBM [8] that will be applied here to incompressible fluids while considering two-phase fluid flows under identical density conditions. In the following, we use non-dimensional variables, as used as in [8]. In the LBM, a modeled fluid, composed of identical particles whose velocities are restricted to a finite set of N vectors $\boldsymbol{c}_i$, is considered. We use the two-dimensional nine-velocity model ($N = 9$)[6] and three particle velocity distribution functions, f_{Ai}, f_{Bi}, and f_{Ci}. The function f_{Ai} is used as an index function for computation of the interface profile in phase X and phase Y, f_{Bi} is used for computation of the pressure and velocity of the two-phase fluid flows, and f_{Ci} is used for computation of the concentration.

The evolution of the particle distribution functions $f_{\sigma i}(\boldsymbol{x},t)$ ($\sigma = A,B,C$) with velocity $\boldsymbol{c}_i$ at point $\boldsymbol{x}$ and at time t are computed with the following equation:

$$f_{\sigma i}(\boldsymbol{x}+\boldsymbol{c}_i\Delta x) - f_{\sigma i}(\boldsymbol{x},t) = \frac{1}{\tau_\sigma}\left\{f_{\sigma i}(\boldsymbol{x},t) - f_{\sigma i}^{\mathrm{eq}}(\boldsymbol{x},t)\right\}, \tag{1}$$

where $f_{\sigma i}^{\mathrm{eq}}$ are equilibrium distribution functions, τ_σ represents non-dimensional single relaxation times, Δx is the spacing of the grid, and Δt is the time step.

The index function $\psi(\boldsymbol{x},t)$, pressure $p(\boldsymbol{x},t)$, velocity $\boldsymbol{u}(\boldsymbol{x},t)$, and concentration $T(\boldsymbol{x},t)$ are defined as follows:

$$\psi = \sum_{i=1}^{9} f_{Ai}, \quad p = \frac{1}{3}\sum_{i=1}^{9} f_{Bi}, \quad \boldsymbol{u} = \sum_{i=1}^{9} f_{Bi}\boldsymbol{c}_i, \quad T = \sum_{i=1}^{9} f_{Ci}. \tag{2}$$

The equilibrium distribution functions $f_{\sigma i}^{\mathrm{eq}}(\boldsymbol{x},t)$ are given by

$$f_{Ai}^{\mathrm{eq}} = H_i\psi + F_i\left(p_0 - \kappa_f\psi\nabla^2\psi\right) + 3E_i\psi\boldsymbol{c}_i\cdot\boldsymbol{u} + E_i\kappa_f\boldsymbol{G}:(\boldsymbol{c}_i\otimes\boldsymbol{c}_i), \tag{3}$$

$$f_{Bi}^{\mathrm{eq}} = E_i\left\{3p + 3\boldsymbol{c}_i\cdot\boldsymbol{u} - \frac{3}{2}|\boldsymbol{u}|^2 + \frac{9}{2}(\boldsymbol{c}_i\cdot\boldsymbol{u})^2\right\} + E_i\kappa_g\boldsymbol{G}:(\boldsymbol{c}_i\otimes\boldsymbol{c}_i), \tag{4}$$

$$f_{Ci}^{\mathrm{eq}} = E_iT\left(1 + 3\boldsymbol{c}_i\cdot\boldsymbol{u}\right), \tag{5}$$

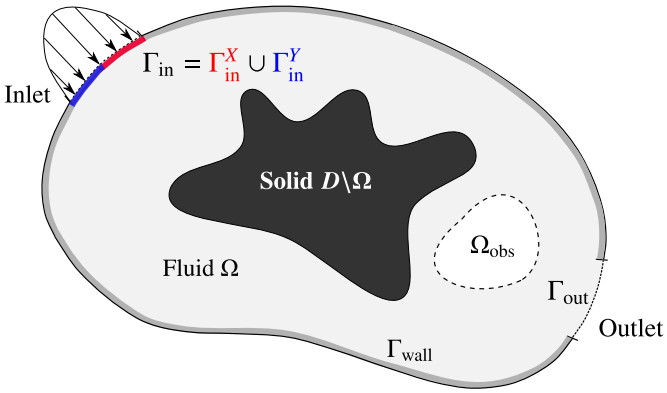


Figure 2: Schematic figure of fixed design domain D in the extraction efficiency maximization problem.

where parameters E_i, H_i, and F_i are defined so that $E_1 = 4/9$, $E_2 = E_3 = E_4 = E_5 = 1/9$, $E_6 = E_6 = E_8 = E_9 = 1/36$, $H_1 = 1$, $H_2 = H_3 = \cdots = H_9 = 0$, $F_1 = -7/3$, and $F_i = 3E_i$ $(i = 2, 3, \cdots, 9)$. κ_f and κ_g are parameters with constant values that determine the width of the interface and the strength of the interfacial tension, respectively. The tensor $\boldsymbol{G}(\boldsymbol{x}, t)$ is defined as follows:

$$\boldsymbol{G} = \frac{9}{2}\nabla\psi \otimes \nabla\psi - \frac{3}{2}|\nabla\psi|^2\boldsymbol{\delta}, \tag{6}$$

where $\boldsymbol{\delta}$ represents the Kronecker delta. In addition, $p_0(\boldsymbol{x}, t)$ is given by

$$p_0 = \psi\bar{T}\frac{1}{1 - b\psi} - a\psi^2, \tag{7}$$

where a, b, and $\bar{T}$ are parameters for determining the profile of index function ψ.

Applying the asymptotic theory to Eqs. (1)–(7), we find that the macroscopic variables, p and $\boldsymbol{u}$, satisfy the Navier-Stokes equations with relative errors of $O(\Delta x^2)$. Note that the pressure is given by $p + (2/3)\kappa_g\nabla|\psi|^2$ in the interface [8]. In addition, the concentration T satisfies the convective-diffusion equation, and the extraction process is represented based on the values of T. The details of the extraction process will be described in the next.

4.2. Topology Optimization Problem

We now formulate the topology optimization problem for the design of a flow channel considering two-phase fluid flows. A schematic diagram of this problem is shown in Fig. 2, with fixed domain D composed of fluid domain Ω and solid domain $D \setminus \Omega$. The inlet boundary condition includes a prescribed velocity, $\boldsymbol{u} = \boldsymbol{u}_{\text{in}}$ at Γ_{in}, and the outlet boundary condition includes a prescribed pressure, $p = p_{\text{out}}$ at Γ_{out}. At the inlet boundary Γ_{in}, the order parameters ψ and concentrations T are respectively set to $\psi = \psi_{\text{in}}^X$ at Γ_{in}^X, $\psi = \psi_{\text{in}}^Y$ at Γ_{in}^Y, $T = T_{\text{in}}^X$ at Γ_{in}^X, and $T = T_{\text{in}}^Y$ at Γ_{in}^Y, where $\Gamma_{\text{in}} = \Gamma_{\text{in}}^X \cup \Gamma_{\text{in}}^Y$ and $\Gamma_{\text{in}}^X \cap \Gamma_{\text{in}}^Y = \emptyset$. In addition, the boundary condition for ψ and T at $\Gamma_{\text{out}} \cup \Gamma_{\text{wall}}$ is set to a Neumann condition, with $\partial\psi/\partial\boldsymbol{n} = \boldsymbol{0}$ and $\partial T/\partial\boldsymbol{n} = \boldsymbol{0}$.

To simultaneously evaluate the extraction efficiency and pressure drop, we define an objective functional, J, based on the weighted sum method, as follows:

$$J = w_1\int_{t_0}^{t_1}\int_{\Gamma} -\boldsymbol{n}\cdot\boldsymbol{u}\left(p + \frac{1}{2}\rho|\boldsymbol{u}|^2\right)\mathrm{d}\Gamma\mathrm{d}t + w_2\int_{t_0}^{t_1}\int_{\Omega_{\text{obs}}}\frac{(T - \langle T\rangle_{\text{in}})^2}{2\langle T\rangle_{\text{in}}^2}\mathrm{d}\Omega\mathrm{d}t, \tag{8}$$

where t_0 and t_1 represent the time step of the LBM calculation, w_1 and w_2 are the weighting parameters, ρ is the fluid density given by $3p$ due to the characteristic of the LBM, and $\langle T\rangle_{\text{in}}$ is the average value of T at the inlet boundary. In the above equation, the second term represents the relative error of T with respect to $\langle T\rangle_{\text{in}}$ in the observation domain, $\Omega_{\text{obs}} \subset D$. The phase X and phase Y concentrations are set to different values, i.e., $T_{\text{in}}^X \neq T_{\text{in}}^Y$. Thus, the second term in Eq. (8) seldom becomes equal to zero during the optimization process. Here, we assume that the extraction process is completely finished when the value of this term does become equal to zero. In addition, since the molecular diffusive coefficient, $k = 1/3\tau_C\Delta x$, is depend on the kind of fluid, the relaxation time τ_C is defined as follows:

$$\tau_C(\psi) = \frac{\psi_{\text{in}}^Y - \psi}{\psi_{\text{in}}^Y - \psi_{\text{in}}^X}\tau_C^X + \frac{\psi - \psi_{\text{in}}^X}{\psi_{\text{in}}^Y - \psi_{\text{in}}^X}\tau_C^Y, \tag{9}$$

where τ_C^X and τ_C^Y represent the relaxation time in phase X and phase Y, respectively.

Based on the above objective functional in Eq. (8), we formulate a topology optimization problem based on our previous research [10], in which the Boltzmann equation is employed when applying a continuous adjoint sensitivity analysis, as follows:

$$\inf_{\gamma\in\mathscr{A}} \quad J[f_{\sigma i};\gamma], \tag{10}$$

$$\text{subject to} \quad \begin{cases} Sh\frac{\partial f_{\sigma i}}{\partial t} + \boldsymbol{c}_i\cdot\nabla f_{\sigma i} = -\frac{1}{\tau_{\sigma i}}\left(f_{\sigma i} - f_{\sigma i}^{\mathrm{eq}}\right) + 3E_i\boldsymbol{c}_i\cdot\boldsymbol{F}_\gamma\delta_{\sigma B} \quad \text{(Boltzmann equation)}, \\ f_{\sigma i}(\boldsymbol{x},t_0) = f_{\sigma i}^0 \quad \text{(initial condition)}, \\ f_{\sigma i}(\boldsymbol{x},t) = f_{\sigma i}^{\mathrm{bc}}(\boldsymbol{x},t) \quad \text{(boundary condition)}, \end{cases} \tag{11}$$

where $\gamma(\boldsymbol{x})$ represents the design variable belonging to the function space $\mathscr{A} = \{\gamma\in L^\infty(D)\,|\,0\leqslant\gamma\leqslant 1 \text{ in } D,\ V_\gamma\leqslant 0\}$, where $V_\gamma(:=\int_D\gamma\mathrm{d}\Omega - V_{\max})$ is the volume constraint that restricts the maximum fluid volume to $V_{\max}$. We let γ vary between zero and unity, with $\gamma=0$ corresponding to a solid domain and $\gamma=1$ to a fluid domain. In Eq. (11), Sh is the Strouhal number, and $f_{\sigma i}^0$ and $f_{\sigma i}^{\mathrm{bc}}$ represent the initial and boundary values for the Boltzmann equation, respectively. We note that the above Boltzmann equation is the so-called *discrete Boltzmann equation* that is not the original equation, since the discrete particle velocities $\boldsymbol{c}_i$ are used. The reason why we use this equation to formulate the optimization problem is that the boundary conditions for adjoint equations can be easily derived based on the adjoint sensitivity analysis.

In addition, $\boldsymbol{F}_\gamma$ is an artificial force, based on the design variable γ, defined as

$$\boldsymbol{F}_\gamma = -\alpha(\gamma)\boldsymbol{u}, \ \text{ where } \ \alpha(\gamma) = \alpha_{\min} + (\alpha_{\max}-\alpha_{\min})\hat{H}(\gamma). \tag{12}$$

In this equation, $\alpha(\boldsymbol{x})$ is the local inverse permeability based on Darcy's law [2], and $\alpha_{\min}$ and $\alpha_{\max}$ are parameters constant value that determine the profile of α. In this study, these parameters are set to $\alpha_{\min}=0$ and $\alpha_{\max}=1.0$, respectively. The profile of $\hat{H}$ is defined as a convex interpolation whose formulation will be described later.

4.3. Level Set-Based Topology Optimization Method

Based on the previous study [11], we use the level set function, $\phi(\boldsymbol{x})$, to express the boundary, $\partial\Omega$, between fluid and solid domains, as follows:

$$\begin{cases} 0<\phi(\boldsymbol{x})\leqslant 1 & \text{for } \boldsymbol{x}\in\Omega\setminus\partial\Omega, \\ \phi(\boldsymbol{x})=0 & \text{for } \boldsymbol{x}\in\partial\Omega, \\ -1\leqslant\phi(\boldsymbol{x})<0 & \text{for } \boldsymbol{x}\in D\setminus\Omega. \end{cases} \tag{13}$$

The level set function has upper and lower limits imposed for the regularization term used to regularize the optimization problem. In addition, $\hat{H}$ is replaced by a smoothed Heaviside function $\hat{H}_\phi(\phi)$ that is defined so that $0\leqslant\hat{H}_\phi\leqslant 1$, as used in the previous study [11].

In a level set-based approach, the optimization problem is replaced with a problem to find an optimal distribution of the level set function. We explore the optimal distribution of ϕ using a time evolution equation, as follows:

$$\frac{\partial\phi(\boldsymbol{x},\varsigma)}{\partial\varsigma} = -K\left\{J'(\boldsymbol{x},\varsigma) - \tau\nabla^2\phi(\boldsymbol{x},\varsigma)\right\}, \tag{14}$$

where $K>0$ is a constant parameter, $\tau>0$ is the regularization coefficient that is set to an appropriate value so that the smoothness of ϕ is maintained during the optimization process, and ς is a fictitious time corresponding to a time step in the optimization. The design sensitivity J' is defined based on the Fréchet derivative.

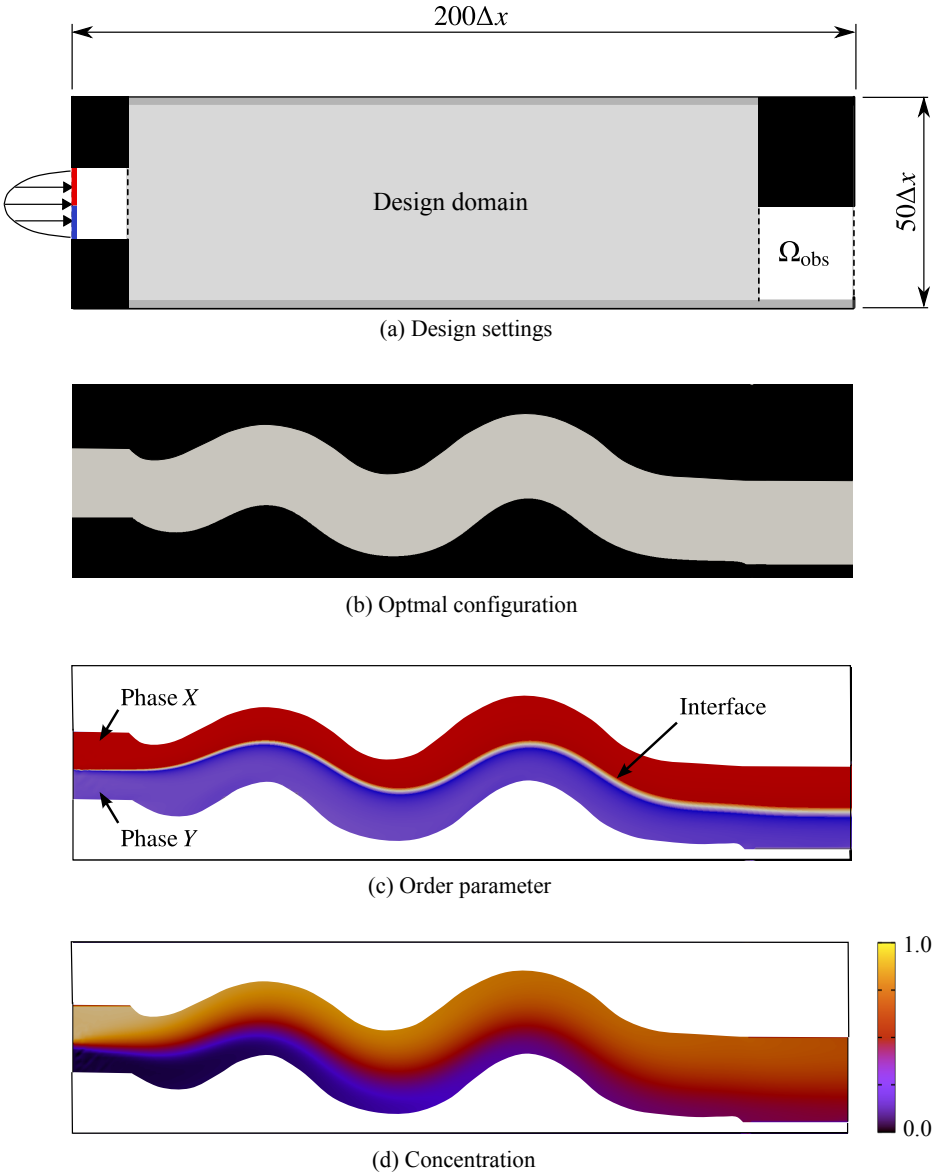
5. Optimization Algorithm

The optimization algorithm of the proposed method is the following.

Step 1. aThe initial level set function is set.

Step 2. bThe two-phase lattice Boltzmann equations are calculated until a steady-state condition is satisfied.

Step 3. cIf the criteria of the objective functional and inequality constraint are satisfied, an optimal configuration is obtained and the optimization is finished, otherwise the design sensitivity is calculated based on the adjoint sensitivity analysis [10].



(a) Design settings

(b) Optmal configuration

(c) Order parameter

(d) Concentration

Figure 3: Design settings, optimal configuration, and the distributions of order parameter and concentration.

Step 4. dThe level set function is updated using the finite element method, after which the optimization procedure returns to Step 2 of the iterative loop.

6. Numerical Example

Here, we provide a numerical example using the proposed method. Figure 3(a) shows the design settings in the extraction maximization problem. The analysis domain is discretized using $200\Delta x \times 50\Delta x$ grids, and the volume constraint is set with $V_{\max} = 0.5$. The optimization parameters are set so that $K = 1$, $\tau = 8.0 \times 10^{-3}$, $\Delta\varsigma = 0.5$, $w_1 = 1.0$, and $w_2 = 0.01$. The initial distribution of the level set function is set to $\phi(\boldsymbol{x}, 0) = \sin(6\pi x/200\Delta x)\sin(2\pi y/50\Delta x)$, so that several holes are present in D at the initial optimization step, $\varsigma = 0$. The Reynolds number is set as $Re = 10$, with the reference length using the inlet width and the reference velocity using the inlet velocity. The kinematic viscosity is given by $\nu = 1/3(\tau_B - 1/2)\Delta x$. The parameters for the two-phase LBM are set so that $\kappa_f = \kappa_g = 1.0 \times 10^{-2}$, $a = 9/49$, $b = 2/21$, $\bar{T} = 0.55$, $T^X_{\text{in}} = 1.0$, $T^Y_{\text{in}} = 0.0$, $\psi^X_{\text{in}} = 1.0$, $\tau^X_C = 0.503$, $\tau^Y_C = 0.553$, and $\psi^Y_{\text{in}} = 0.5$. Thus, the Schmidt number and the Péclet number are given by $Sc = 10$ and $Pe = 100$, respectively.

As shown in Fig. 3(b), a sinuous channel is obtained as an optimal configuration, a suitable form that sufficiently diffuses the concentration of the two phases, whose distribution is shown in Fig. 3(d). In addition, we can confirm that the interface between phase X and phase Y is expressed by the order parameter value, whose

distribution is shown in Fig. 3(c). We note that the obtained optimal configuration is similar to the results of previous studies [5,12], in which the interface effect is not treated while the concentration is calculated based on the convective-diffusion equation.

7. Conclusion

This paper proposed a new topology optimization method using a two-phase LBM for the design of the channel configuration in a microchannel device. In this research, the extraction process was modeled using concentration values that are governed by a convective-diffusion equation. The presented method was applied to an extraction maximization problem and a numerical example demonstrated the validity of the proposed method.

8. Acknowledgments

This work was supported in part by a grant for JSPS KAKENHI, Grant Number 26820032.

9. References

[1] O. Sigmund and K. Maute, Topology optimization approaches, *Structural and Multidisciplinary Optimization*, 48 (6), 1031-1055, 2013.

[2] T. Borravall and J. Petersson, Topology optimization of fluids in Stokes flow, *International Journal for Numerical Methods in Fluids*, 41 (1), 77-107, 2003.

[3] F. Okkels and H. Bruus, Scaling behavior of optimally structured catalytic microfluidic reactors, *Physical Review E*, 75 (1), 016301, 2006.

[4] C.S. Andreasen, A.R. Gersborg and O. Sigmund, Topology optimization of microfluidic mixers, *International Journal for Numerical Methods in Fluids*, 61 (5), 498-513, 2009.

[5] D. Makhija, G. Pingen, R. Yang and K. Maute, Topology optimization of multi-component flows using a multi-relaxation time lattice Boltzmann method, *Computers and Fluids*, 67, 104-114, 2012.

[6] S. Succi, *Lattice Boltzmann Equation for Fluid Dynamics and Beyond*, Oxford University Press, New York, 2001.

[7] P. Znidarsic-Plazl and I. Plazl, Steroid extraction in a microchannel system–mathematical modeling and experiments, *Lab on a Chip*, 7, 883-889, 2007.

[8] T. Inamuro, R. Tomita and F. Ogino, Lattice Boltzmann simulations of drop deformation and breakup in shear flows, *International Journal of Modern Physics B*, 17 (1,2), 21-26, 2003.

[9] M.M. Tekitek, M. Bouzidi, F. Dubois and P. Lallemand, Adjoint lattice Boltzmann equation for parameter identification, *Computers and Fluids*, 35 (8,9), 805-813, 2006.

[10] K. Yaji, T. Yamada, M. Yoshino, T. Matsumoto, K. Izui and S. Nishiwaki, Topology optimization using the lattice Boltzmann method incorporating level set boundary expressions, *Journal of Computational Physics*, 274, 158-181, 2014.

[11] T. Yamada, K. Izui, S. Nishiwaki and A. Takezawa, A topology optimization method based on the level set method incorporating fictitious interface energy, *Computer Methods in Applied Mechanics and Engineering*, 199 (45-48), 2876-2891, 2010.

[12] D. Makhija and K. Maute, Level set topology optimization of scalar transport problems, *Structural and Multidisciplinary Optimization*, 51 (2), 267-285, 2014.