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Improved pillar shape for deterministic lateral displacement separation method to maintain separation efficiency over a long period of time

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ABSTRACT

Deterministic lateral displacement (DLD) separation utilizes streamlines produced by an array of pillars, which determine the critical diameter. However, particle clogging often occurs at the gaps between the pillars and alters the streamlines. This leads to a drastic reduction in the separation efficiency. In this study, a topology optimization technique has been applied to design a new pillar shape. This will allow the gap between the pillars to be increased in order to minimize particle clogging without affecting the originally designed critical diameter, thereby maintaining higher separation efficiency over a long period. Experimental investigations revealed that a DLD device with the optimized pillar forms a smaller clogging region over a longer period of time than DLD devices with circular- or triangular-shaped pillars. In the DLD device with the optimized pillars enables to maintain 92.2% separation efficiency in displacement mode over 30 min, whereas in circular pillars the separation efficiency in displacement mode progressively reduces to 77%. This result leads to the conclusion that the microfluidic device with the optimized pillar shape can provide consistent separation efficiency for a long period of time. It is believed that this device could be used for separating rigid particles as alternative way to produce super-monodispersed micro-particles with affordable cost.

1. Introduction

Cell separation is an important technique in the fields of biology and medical sciences, where it finds several applications in specialties such as cell biology, diagnostics, and therapeutics [1–3]. The separation of a target cell from a heterogeneous population of various cells is an essential preparatory step for individual cell study. This separation leads to a better understanding of cells for determining the effects of drugs and for studying environmental issues [4–7]. Deterministic lateral displacement (DLD) is a size-based passive separation technique that affords relatively high separation resolution compared to other separation techniques [8–12]. It has been used for separating various cells such as blood cells [13–15], cancer cells [16], droplets [17], parasites [18], and deformable particles [19]. However, this separation method is limited owing to its reliance on a fluid streamline produced by an array of pillars, and the gap between the pillars is very susceptible to clogging [9,20]. Clogging alters the streamline, resulting in a drastic reduction in the efficiency of particle or cell separation with time. To overcome clogging, it is necessary to increase the gap between the pillars (g) [9]. However, this gap is linearly related to the critical diameter that determines the particle motions (zigzag mode and displacement mode); therefore, the extent to which the gap can be increased is limited.

Several methods have been proposed for increasing the efficiency of particle or cell separation. Beech et al. introduced a tunable DLD separation method that involves stretching the DLD device to reduce clogging [21]. Lubbersen et al. reported that the chances of clogging can be reduced by increasing the Reynolds number [28,29]. Loutherback et al. reported numerical and experimental studies that show that triangular pillars produced a greater gap between the pillars than circular ones [20]. Triangular pillars generate a compressed streamline around their edge and create an asymmetric velocity profile in the gaps. This affords a smaller critical diameter for a given gap between the pillars compared to circular pillars. In other words, for a given critical diameter, triangular pillars allow for a wider gap than circular pillars, reducing the possibility of particle clogging. However, from an engineering viewpoint, it would be more beneficial to find an optimized pillar by using a well-established optimization technique so that a DLD device performs best under given constraints.

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In the present study, topology optimization has been used to determine the optimal pillar shape for achieving a wide gap between pillars for a given critical diameter. Topology optimization is a technological concept used to determine the optimum structure for a given objective function under defined constraints. It has several applications, including solid mechanics, acoustics, fluid mechanics, and microfluidics [22–26]. In the case of a microfluidics device, researchers optimized micromixer [25,30], micropump [31] and microvalve [32] using topology optimization; however, a separation device has not yet been reported. The primary purpose of this study was to determine an optimized pillar shape for DLD separation that produces a maximum asymmetric velocity profile in the given gap between the pillars under given constraints. Increasing the gap between the pillars reduces clogging and facilitates the maintenance of high separation efficiency over a long period.

2. Material and methods

2.1. Working principle of DLD separation

The working principle of DLD separation is shown in Fig. 1(a). The red line indicates the streamlines produced by the array of pillars. The main concept of separation is to determine the first streamline (critical radius: β), as shown in Fig. 1(a). As shown in Fig. 1(b), if the radius of a particle is smaller than β, the particle travels in zigzag mode. However, if its radius is larger than β, it travels in displacement mode [8,9]. β can be determined by the three parameters described in Eq. (1): g (gap between the pillars), ε (row shift fraction), and $\boldsymbol{u}(x,y)$ (fluid velocity) [8]. ε is defined as the row shift distance of pillars from the lateral direction ($\Delta\lambda$) divided by the distance between the center of the pillars (λ). As shown in Fig. 1(a), the fluid flux from the pillar to β can be replaced by the fluid flux from the pillar to $\varepsilon\lambda$. However, because no fluid flux should exist inside the pillars, the fluid flux in β can be represented by ε and g from Eq. (1). In this paper, D_c (critical diameter) is defined as two times β.

$$\varepsilon = \Delta\lambda/\lambda$$

$$|\boldsymbol{u}(x,y)| \cong u_x(x,y)(u_y(x,y) \cong 0)\ [\mathrm{m/s}]$$

$$Q = \varepsilon\int_0^g u_x(x,y)dy = \int_0^{\beta sy} u_x(x,y)_{sy}dy$$
$$= \int_0^{\beta asy} u_x(x,y)_{asy}dy(\beta_{sy} > \beta_{asy})\ [\mathrm{m^2/s}]$$

$$D_c = 2\beta\ [\mathrm{m}] \tag{1}$$

To reduce the clogged regions without influencing D_c, the gap between the pillars should be increased. One approach to increase the gap is to increase the degree of asymmetricity of the velocity profile while maintaining D_c. Fig. 1(c) shows a comparison of the (left) imaginary symmetric velocity profile and (right) asymmetric velocity profile for the same gap (g), row shift fraction (ε), and total fluid flux between the pillars. The asymmetric velocity profile has a smaller D_c than the symmetric velocity profile owing to the greater fluid flux near the pillar. This implies that g can be further increased to prevent or minimize particle clogging between the pillars without influencing the designed D_c, as the asymmetric ratio of the velocity profile increases. In this study, the topology optimization technique has been applied to determine the optimal shape of the pillars that produces the maximum degree of asymmetric ratio in the velocity profile between the pillars.

2.2. Topology optimization

Topology optimization is a mathematical approach for optimizing the design domain of a material, the layout for given boundary conditions, and the constraints to determine the best desirable design. In this study, topology optimization was used to determine the optimal pillar shape under given constraints that would produce a maximum asymmetric velocity profile between the pillars. This would increase the gap between the pillars while maintaining D_c as designed. The commercial software COMSOL Multiphysics (Comsol, USA) was used for the simulations. Several assumptions had been made before the simulations, namely, that the fluid flow is laminar owing to its microscale and incompressible. Furthermore, the steady-state condition was applied to the NSE (Navier–Stokes equations) as the fluidic properties do not change over time. The fluid flow in the channel is therefore described by the steady-state NSE with an artificial porosity term (Darcy term; Eq. (2)) to perform topology optimization. The Darcy term will determine the porosity value in the given design domain. Constant parameters that have been used in the simulation are attached in Supplementary section (see Table S1, Supplementary Information).

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nabla\cdot\eta(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) - \alpha(\gamma)\mathbf{u} \tag{2}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{3}$$

$$(\text{Pressure drop} = p_2 - p_1,\ u_2 = u_1)$$
$$(\text{Pressure} - \text{driven periodic condition; 2 and 1 refer to inlet and outlet parts})$$
$$(p_a = p_b,\ u_a = u_b)\ (\text{Periodic flow condition; } a \text{ and } b \text{ refer to boundary regions}) \tag{4}$$

$$Da = \frac{\eta}{\alpha_{max} l^2} \tag{5}$$

$$\alpha(\gamma) \equiv \alpha_{max}\frac{q(1-\gamma)}{q+\gamma} \tag{6}$$

Eq. (2) describes the governing equation for topology optimization. The governing equation includes the NSE with the Darcy term ($\alpha(\gamma)\mathbf{u}$) (ρ is the density of the fluid; η, the dynamic viscosity of fluid; $\alpha(\gamma)$, the porosity term; $\mathbf{u}(\mathbf{u} = [\mathrm{u}, \mathrm{v}]^{\boldsymbol{T}})$, the velocity field; and p, the pressure). The Darcy term ($\alpha(\gamma)\mathbf{u}$) applies to a porous medium, which is linear to inverse permeability. Here, γ is a design parameter that has a value of 0 or 1. When $\gamma = 1$, the $\alpha(\gamma)$ term (Darcy term) vanishes from the governing equation (Eq. (1)), leaving only the NSE. The disappearance of the Darcy term indicates the fluid part in the design domain. When $\gamma = 0$, the $\alpha(\gamma)$ term exists in the governing equation; this indicates the solid part in the design domain. From Eq. (6), $\alpha(\gamma)$ is linear to α_{max} and is dependent on the Darcy number (Da) (Eq. (5)). Therefore, when Da is small, α_{max} has a larger value and is defined as the smaller permeable solid part in the governing equation. Therefore, the Darcy approximation is necessary in fluidic topology optimization. This method has been widely used in other papers [24,25,27]. Here, q stands for a real and positive parameter used to tune the shape of $\alpha(\gamma)$.

Eq. (3) is a continuity equation that indicates that the fluid is incompressible. Periodic boundary conditions are defined by Eq. (4). The periodic condition indicates the same pressure and velocity in the given boundary condition.

In Eq. (5), l denotes the characteristic length of the system. Da is the ratio of the viscous friction force to the porous friction force that determines the solid and fluid part of the structure numerically.

2.3. Device fabrication

The device was microfabricated by UV lithography and a polydimethylsiloxane (PDMS) replica molding technique. A 1-μm-