

Universal correlation for the critical diameter of deterministic lateral displacement devices with polygonal posts

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(Dated: 11 June 2024)

Deterministic lateral displacement (DLD) is a microfluidic technique that utilizes a specific array of micro-posts to separate cells or particles larger and smaller than a critical diameter. The critical diameter depends on the shape of the posts, the gap between the posts, and the relative shift between the adjacent rows of posts. Here, we present an experimental and numerical investigation to elucidate the functional dependence of the critical diameter of DLD arrays with polygonal posts on the geometric parameters. Based on simulations of fluid flow through DLD devices with varying geometric parameters, we first derived a correlation to predict the critical diameter of DLD arrays with polygonal post shapes having arbitrary number of sides. We then used a novel experimental approach, wherein we coupled different DLD arrays with an upstream droplet generator to flow droplets of varying sizes and estimate the critical diameter. The critical diameter predicted by the correlation based on simulations compares well with our experimental data and with data available in the literature. The universal correlation for critical diameter presented here can help design and optimize DLD devices with polygonal posts.

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I. INTRODUCTION

The ability to precisely position and separate particles at the micrometer and nanometer scale holds the key to advancements in chemical analysis, diagnostic techniques, and advanced material engineering. Numerous microfluidic methods for particle separation exist, which can be broadly classified as passive and active methods and their combinations. Passive methods utilize specific flow features and particle interaction for separation and sorting. Examples of passive methods include pinched flow fractionation,¹ inertia and dean flow fractionation,² micro vortex manipulation,³ and Zweifach-Fung effect.⁴ In contrast, active methods, such as dielectrophoresis⁵ and fluorescence-activated cell separation,⁶ rely on applying external forces such as electric, magnetic, and acoustic forces to effect particle separation. Typically passive particle separation methods are preferred over active methods as external forcing can alter the particle and cell properties.^{7,8}

Deterministic lateral displacement (DLD) has emerged as a promising approach for passive particle separation and sorting. DLD is a size-based separation and sorting technique, introduced by Huang et al.,⁹ which utilizes a specific array of micro-posts to separate particles larger and smaller than a critical diameter (D_C). A typical DLD device consists of an array of micro-posts, as illustrated in Fig. 1. The geometry of a DLD array is characterized by the center-to-center distance λ , gap between the posts g , side length of the post (or diameter for circle) D . Each row of the micro-posts is shifted laterally by a distance of $\Delta\lambda$ with respect to the upstream row.

To describe the working principle of the DLD array, we consider an array with a periodicity of $n = \lambda/\Delta\lambda = 3$, as shown in Fig. 1. Now, as described by Huang et al.,⁹ the total fluid flux through each gap can be divided into n streams of laminar flow with equal fluid rates, as illustrated in Fig. 1. Moreover, each streamlines are separated by stall lines. As the lanes go through the gaps, their positions change periodically, making them return to their initial position after n rows. The width of the first streamlane (the right lane with respect to the post), denoted by β , governs the particle sorting. If the hydrodynamic center of the flowing particle lies within the width of the first streamlane, such as the smaller (red) particle in Fig. 1, it continues to follow that lane downstream. Consequently, such a particle moves in a zigzag mode, returning to the same lateral position after traveling n rows of posts. On the other hand, if the hydrodynamic center of the particle lies outside the width of the

first streamline, the particle gets displaced to the adjacent lane while negotiating a post, as illustrated by larger green particles in Fig. 1. Such a particle experiences a lateral shift each time it interacts with a post. This mode of particle motion is termed as the displacement mode. In displacement mode, the particle is displaced by an angle $\alpha = \tan^{-1}(1/N)$ to the mean flow direction. An alternative explanation of the working principle of a DLD array has been given by Kim et al.¹⁰. They showed that the pillar array geometry distorts the fluid flow, such that particle trajectories do not necessarily follow the periodicity or symmetry of the array, generating trajectories with migration angles that can have values between 0 and the array angle (α).

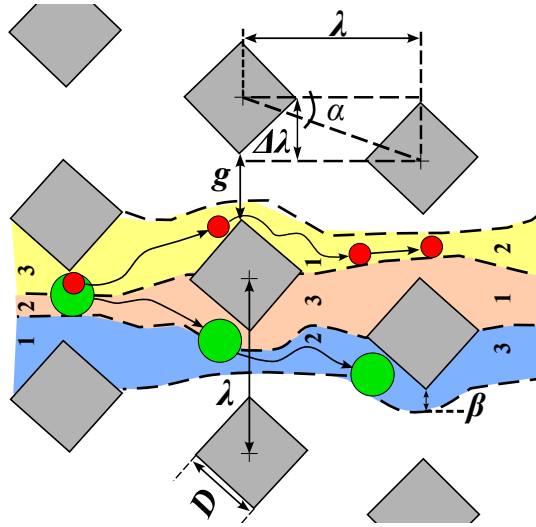


FIG. 1. Schematic of a DLD array showing the geometric parameters: center-to-center distance λ ; side length of the post D ; incremental displacement $\Delta\lambda$ in each successive row, making the row shift fraction, $\epsilon = \Delta\lambda/\lambda$; and displacement angle, $\alpha = \tan^{-1}(\epsilon)$. Shown here is a DLD array with $\epsilon = 1/3$. The streamlanes 1 – 3 carry equal flow rate. The red and green particles indicate the trajectories of droplets following zigzag and displacement modes, respectively.

The critical diameter, D_C , above which a particle flows in the displacement mode, is given by twice the width of the first streamlane (β), $D_C = 2\beta$. For circular posts, Davis et al.¹¹ proposed an empirical correlation for D_C in terms of the gap between two adjacent posts and the row shift fraction $\epsilon = \Delta\lambda/\lambda = 1/N$, given by

$$D_C = 1.4g\epsilon^{0.48}. \quad (1)$$

This correlation facilitates the design of DLD arrays with circular posts, wherein parameters g and ϵ are tuned to obtain the desired critical diameter. Although strictly applicable for circular posts, Eq. (1) has also been used as an approximate guideline for designing DLD arrays with non-circular post shapes.^{12,13} However, the critical diameter of the DLD array strongly depends on the post shape. For example, Louthierback et al.¹⁴ showed using simulations and experiments that DLD arrays with triangular posts have significantly lower critical diameter than that of circular posts for the same gap g and row shift fraction ϵ . Similarly, through simulations and experiments of a DLD array with rotated square posts, Fandi et al.¹⁵ demonstrated a lower critical diameter than similar DLD array with circular posts. Despite the benefits of polygonal posts for DLD separation, currently, no correlation exists that accurately predicts the critical diameter. Therefore, for the design of such arrays, one must resort to numerical simulations, as demonstrated by Louthierback et al.,¹⁴ to estimate the critical diameter.

In this paper, we present a detailed numerical and experimental investigation to characterize the dependence of the critical diameter (D_C) of DLD arrays with polygonal posts on the geometric features. In particular, we present a generalized correlation to determine D_C for polygonal posts with arbitrary number of sides and its validation with experimental data. We begin by describing fluid flow through a DLD array with polygonal-shaped posts using numerical simulations. Thereafter, we present the calculation of D_C from the simulation data and the development of the correlation for D_C . Next, we present a novel experimental approach to couple DLD arrays with a droplet generator to flow droplets of varying sizes and precisely estimate the critical diameter. Finally, we validate the correlation for D_C with our experimental data as well as the data available in the literature.

II. NUMERICAL SIMULATIONS

In general, the particle separation process in DLD and its critical diameter depends on various physical parameters which can be grouped into the following three categories: (i) mean flow velocity u , (ii) geometrical parameters such as diameter or side-length of the post D , gap between two posts g , center-to-center distance λ , row shift in successive rows $\Delta\lambda$ and the number of sides of the polygonal post n , and (iii) physical properties of the fluid such

as density ρ and dynamic viscosity μ . Therefore, the critical diameter D_C for a DLD array with polygonal posts can be expressed as,

$$D_C = f(u, g, \lambda, \Delta\lambda, D, \rho, \mu, n). \quad (2)$$

This relationship can be expressed in dimensionless form as

$$\frac{D_C}{g} = F\left(\text{Re}, \epsilon, n, \frac{D}{g}\right). \quad (3)$$

where $\epsilon = \lambda/\Delta\lambda$ is row shift fraction and $\text{Re} = \rho u D / \mu$ is the Reynolds number. Typically, DLD arrays operate at low values of Reynolds number. At low Reynolds numbers, the flow field is independent of the Reynolds number. Hence, the effect of Reynolds number on D_C can be neglected. Therefore, Eq. (3) simplifies to

$$\frac{D_C}{g} = F\left(\epsilon, n, \frac{D}{g}\right). \quad (4)$$

To find the functional dependence of D_C/g on ϵ , D/g , and n , we performed 2D computational fluid dynamics (CFD) simulations for varying values of ϵ , D/g , and n . We performed 2D simulations because comparison with 3D simulations showed less than 5% variation in the calculated critical diameter (see supplementary material). We simulated seven regular polygonal configurations: (a) triangular ($n = 3$), (b) square ($n = 4$), (c) pentagonal ($n = 5$), (d) hexagonal ($n = 6$), (e) heptagonal ($n = 7$), (f) octagonal ($n = 8$), and (g) circle ($n \rightarrow \infty$). For each n , we performed simulations for ϵ varying between 1/150 to 1/3. Moreover, to elucidate the dependence of D_C/g on the post size (D/g), we varied D/g from 0.2 to 2. For this, we fixed the side length of the post (or diameter for the circle) to be 20 μm and varied the gap between 10 to 200 μm .

Figure 2 shows a representative computational domain for DLD array with rotated square micro-posts. We considered a small portion of the actual DLD device as a computational domain consisting of a 10×10 periodic array of posts. The simulations were performed by solving the 2D continuity and Navier-Stokes equations for steady, incompressible flow using the COMSOL Multiphysics software. We used a normal inflow velocity boundary condition at the inlet, and a constant pressure boundary condition was applied at the outlet. The no-slip boundary condition was applied on the walls of polygonal posts. We used periodic

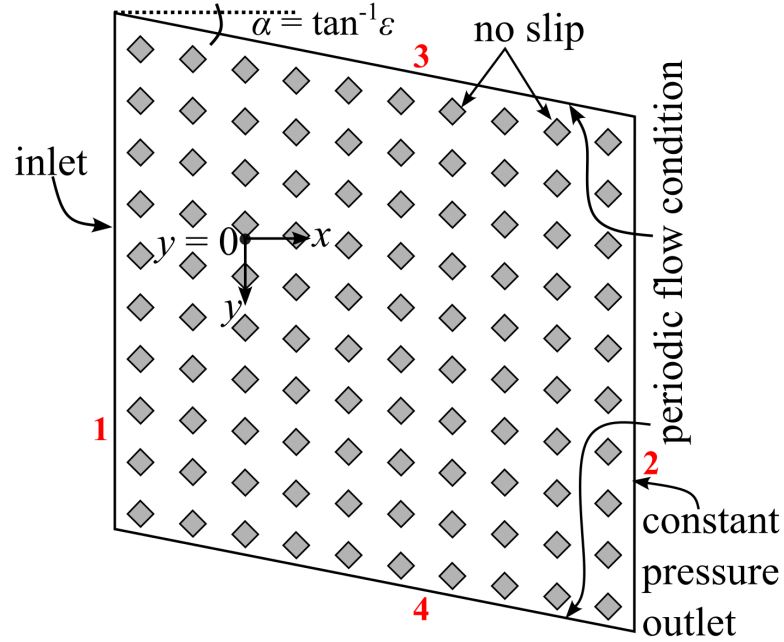


FIG. 2. Schematic of the computational domain consisting of a 10×10 array of posts. Periodic boundary conditions were applied on the top and bottom boundaries (boundaries 3 and 4), and no-slip boundary conditions were applied on the post walls. A normal inflow velocity boundary condition was applied at the inlet (boundary 1) and constant pressure boundary condition was applied at the outlet (boundary 2)

flow conditions on the sidewall of the computational domain. The mathematical expressions for the boundary conditions are provided in the supplementary material. The sample fluid was taken as water with a density of 997.1 kg m^{-3} and a dynamic viscosity of $8.91 \times 10^{-4} \text{ Pa s}$. We performed a grid-independence test to identify the optimum mesh size and thereafter used the same mesh parameters for all the simulations.

In Figs. 3(a)-(g), we compare the computed streamlines for seven DLD arrays with polygonal posts varying in the number of sides. For polygons with an even number of sides and circular posts (Figs. 3(b), (d), (f), and (g)), the symmetry of the adjacent posts results in symmetrical streamlines. In contrast, Figs. 3(a), (c), and (e) show asymmetry in streamlines for polygonal posts with an odd number of sides ($n = 3, 5$, and 7). This asymmetry arises due to the inherent geometric asymmetry of the triangle, pentagon, and heptagon-shaped posts, causing the velocity profile between the posts to shift towards the sharp boundary, as depicted in Fig. 3(h). Although polygonal posts with an even number of sides can also exhibit flow asymmetry if the adjacent posts are rotated relative to each other,¹⁶ this study limits the analysis to DLD arrays without such rotation. Additionally, Fig. 3(h) shows that

as the number of sides n of the polygonal posts increases, the velocity profile between the gaps approaches that of a DLD array with circular posts.

Having computed the velocity profile for steady flow between adjacent posts (Fig. 3(h)), we used the method suggested by Inglis et al.¹⁷ to calculate the critical diameter, D_C based on the width of the first streamline next to a post (see Fig. 1). To illustrate this procedure,

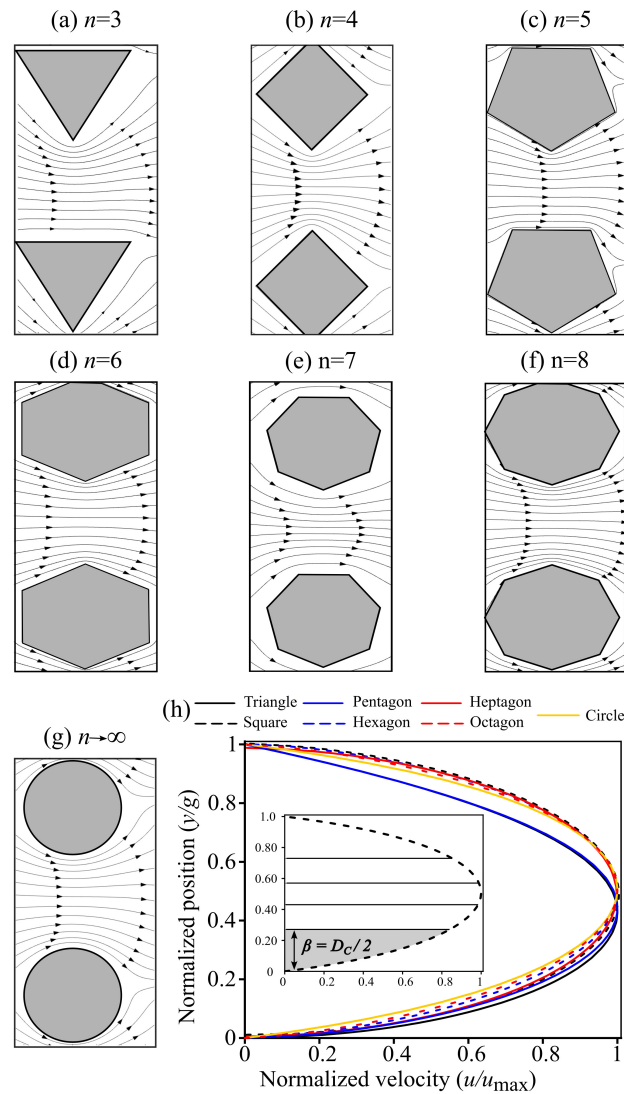


FIG. 3. Comparison of flow streamlines in DLD devices with different polygonal posts. (a) triangular ($n = 3$), (b) square ($n = 4$), (c) pentagonal ($n = 5$), (d) hexagonal ($n = 6$), (e) heptagonal ($n = 7$), (f) octagonal ($n = 8$), and (g) circular ($n \rightarrow \infty$). For these simulations, the row shift fraction, $\epsilon = 0.20$. (h) Comparison of horizontal velocity (u/u_{max}) profiles of different polygonal posts with row shift fraction is $\epsilon = 0.20$. Sharp vertex with an adjacent flat edge creates asymmetric flow conditions, as observed in (a), (c), and (e), and as a result, the flow profiles are shifted towards the vertex, as shown in (h). On the other hand, for polygons with an even number of sides, the flow is relatively symmetrical, as seen in (b), (d), (f), and (g).

we consider the velocity profile between square posts, as shown in the inset of Fig. 3(h). The width of the streamlane β is such that the flow rate between the post edge ($y = 0$) and $y = \beta$ is $\epsilon (= 1/N)$ times the net flow rate between the gap of two adjacent posts, with n representing the periodicity of the device; for a given pair of posts, $y = 0$ is the bottom most point of the top post, as shown in Fig. 2. That is, β is given by,

$$\int_0^\beta u(y) dy = \epsilon \int_0^g u(y) dy. \quad (5)$$

The width of the first stream β , calculated for DLD array with square posts with a row shift fraction of, $\epsilon = 0.20$, is shown in the inset of Fig. 3(h). Now, if the hydrodynamic center of a particle is within the first streamlane's width, it continues downstream in a zigzag mode. However, if the center lies outside this width, the particle is displaced to the adjacent lane during post-interaction, leading to a lateral shift and displacement mode. Therefore, the critical radius of a particle above which displacement mode is observed equals the width of the first streamlane (β), making the critical diameter $D_C = 2\beta$.

The above discussion on the calculation of the critical diameter of DLD arrays assumes

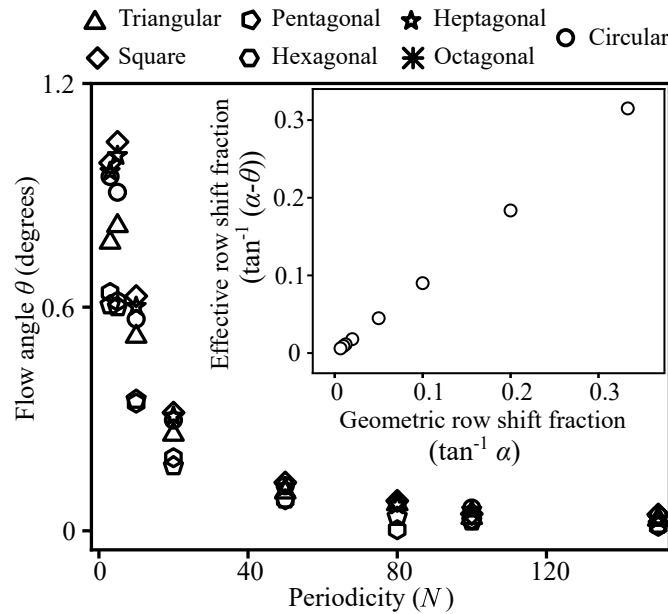


FIG. 4. Variation of the average flow angle (θ) with the periodicity of DLD devices with different polygonal posts. As the periodicity increases, the geometric angle ($\alpha = \tan^{-1}(1/N)$) decreases and hence flow becomes relatively horizontal. The inset shows the variation of the effective row shift fraction ($\tan^{-1}(\alpha - \theta)$) with the geometric row shift fraction ($\tan^{-1} \alpha$).

that the average flow is along the horizontal (x -direction). However, the periodic boundary conditions do not constrain the flow to be horizontal. Consequently, as shown by Vernekar et al.,¹⁸ the average flow makes an angle $\theta = \tan^{-1}(v_{\text{avg}}/u_{\text{avg}})$ with the horizontal. In Fig. 4, we plot the variation of flow angle (θ) with periodicity ($N = 1/\epsilon$) of DLD arrays with polygonal posts. The average flow angle decreases with an increase in periodicity. While the flow angle is predominantly horizontal ($\theta \approx 0^\circ$) for high values of periodicity, the effect of the flow tilt can not be neglected for DLD arrays with smaller periodicity. To account for the flow tilt, we consider an effective row shift fraction given by $\tan^{-1}(\alpha - \theta)$. The dependence of the effective row shift fraction on the geometric row shift fraction is shown in the inset of Fig. 4. The effective row shift fraction is more or less the same as the geometric row shift fraction except for higher values of the row shift fraction, where the flow angle is non negligible. Hereafter, in our simulation results, ϵ represents this effective row shift fraction ($\tan^{-1}(\alpha - \theta)$). Correspondingly, to calculate the critical diameter we used the effective row shift fraction in Eq. (5).¹⁹

Our simulations showed a weak dependence of D_C/g on the post size (D/g) which is presented in the supplementary material. This suggests that $D_C/g = F(\epsilon, n)$. In Fig. 5(a), we present the variation of calculated D_C/g with the number of sides of the polygonal posts n for varying row shift fraction ϵ . Figure 5(a) shows that for the given number of sides (n), the critical diameter (D_C) increases with row shift fraction (ϵ). Moreover, for given ϵ , D_C/g increases at a different rate for odd and even values of the number of sides of polygon n . Figure 5(b) shows that $\ln(D_C/g)$ varies linearly with $\ln \epsilon$, and the slope m varies with n . This suggests a power-law relation of the form

$$\frac{D_C}{g} = A\epsilon^m, \quad (6)$$

where the exponent m depends on the number of sides of the polygon, n .

To elucidate the dependence of the exponent m on the number of sides n of the polygonal posts, in the inset of Fig. 5(b), we present the variation of m with n . We observe that the m decreases with increasing values of n , attaining an asymptotic value of 0.57 for $n \rightarrow \infty$ which corresponds to the circular post. However, the exponent m follows different trends for odd and even values of n . We fitted a function of the form, $m = 0.57 + a/n^b$, to the fitted values

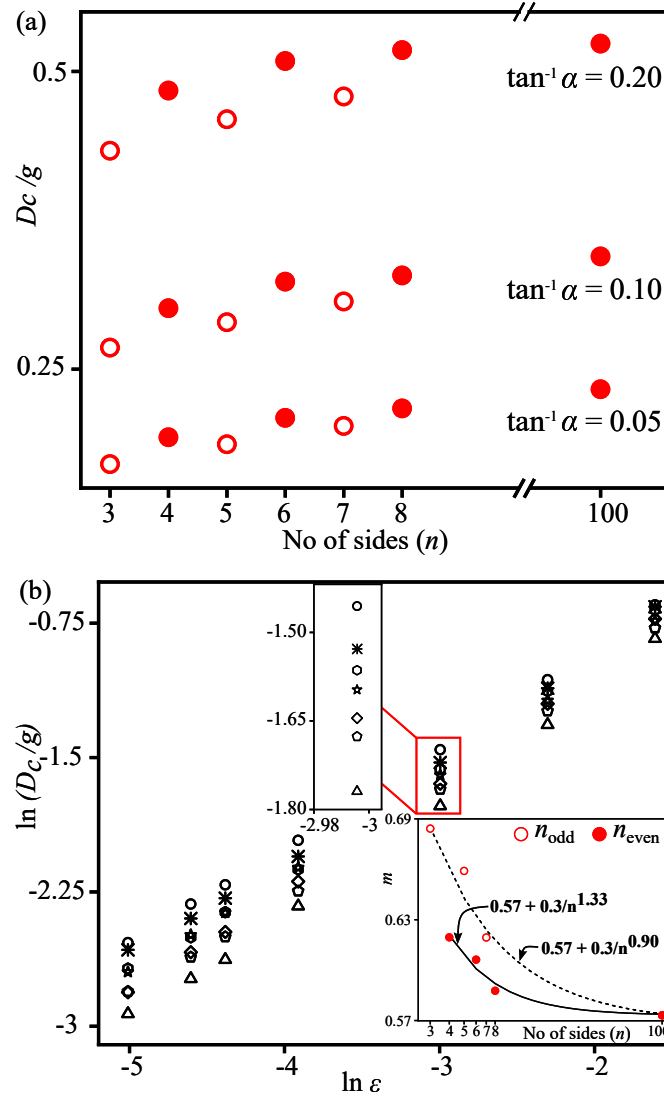


FIG. 5. (a) Variation of critical diameter with the number of sides of a polygonal post for geometric row shift fraction $\tan^{-1} \alpha = 0.05, 0.10, 0.20$. As the number of sides increases, the critical diameter also increases, approaching that for DLD array with circular post. (b) shows that $\ln(D_c/g)$ varies linearly with $\ln \epsilon$, and the slope m varies with the number of sides n of the polygonal posts. This suggests a power-law relation of the form $D_c/g = Ae^m$. The inset of (b) shows the coefficient m follows different trends for polygonal posts with an odd or even number of sides.

of m . As shown in the inset of Fig. 5(b), $m = 0.57 + 0.3/n^{1.33}$ reasonably approximates the variation of exponent m with n for even values of n .

Compared with the exponents m for even number of polygonal sides n , the exponent m for odd values of n decays slowly upon increasing n . In other words, upon increasing n , the critical diameter of DLD array with polygonal posts approaches that for circular posts slower for odd values of n compared with even values of n . This difference can be attributed

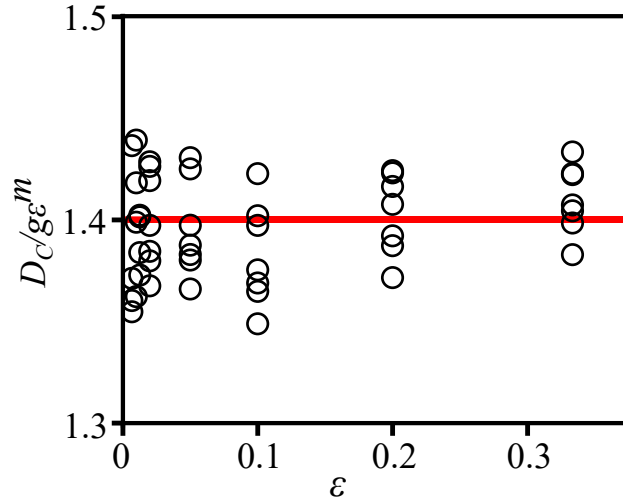


FIG. 6. Comparison of the critical diameters obtained from the simulations and those predicted from Eq. (7) for different values of g and ϵ . All the simulation data collapsed around the horizontal line at 1.4, suggesting good agreement between predicted and simulated critical diameter values.

to the fact that the velocity profile between the posts for odd values of n is asymmetric and approaches to that for circular posts on increasing n , relatively slowly compared with that for even values of n . As shown in the inset of Fig. 5(b), $m = 0.57 + 0.3/n^{0.90}$ reasonably approximates the variation of exponent m with n , for odd values of n .

Unlike the exponent m , the coefficient A shows a weak dependence on the number of sides n of the polygonal posts. Plotting $D_C/g\epsilon^m$ versus ϵ , as shown in Fig. 6, yields a constant value of $A = 1.4$ for polygonal and circular posts. Therefore, the final correlation for the critical diameter can be written in a convenient form as

$$\frac{D_C}{g} = 1.4\epsilon^m, \quad m = 0.57 + \frac{0.30}{n^p}, \quad (7)$$

where $p = 0.90$ and 1.33 for odd and even values of n , respectively.

Compared with the correlation given by Davis et al.,¹¹ Eq. (1), the developed correlation incorporates the variation of the critical diameter due to flow tilt associated with anisotropic permeability¹⁸ and the effect of post-shape on critical diameter by including the number of sides of polygon n in Eq. (7), making it possible to predict the critical diameter for polygonal posts with an arbitrary number of sides. In Fig. 6, we plot $D_C/g\epsilon^m$ versus ϵ to check the validity of Eq. (7). Note that Eq. (7) predicts the exponent $m = 0.57$ for DLD arrays with

circular posts, whereas the correlation of Davis et al.¹¹ has $m = 0.48$. This difference can possibly be due to limited experimental data for circular posts used by Davis et al.¹¹ In contrast, our correlation is based on extensive simulation data with an effective row shift fraction and is then validated with a large experimental dataset (see Section III).

Overall, based on the variation of critical diameter with ϵ, g, n shown in Fig. 5, and by the correlation, we draw the following conclusions. Firstly, the critical diameter increases with the number of sides of the polygonal post for all values of the row shift fraction or the periodicity of the DLD array. Therefore, for any given value of g and ϵ , triangular posts give the smallest critical diameter. That is, the triangular posts are most suitable for the separation of smaller particles. On the other hand, circular posts ($n \rightarrow \infty$) yield the largest critical diameter for the given values of gap and the row shift fraction. Secondly, for a given post shape and gap, the critical diameter can be decreased by increasing the periodicity of the DLD array (reducing the row shift fraction ϵ). These observations are consistent with the experimental work of Loutharback et al.,¹⁴ who first demonstrated the use of triangular posts in DLD devices to achieve a smaller critical diameter. We note that the correlation given by Eq. (7) is based on the assumption that the flow field is unperturbed by the flow of particles through the DLD device. However, the flow of large particles with diameters comparable to the gap between the posts can alter the flow field. Therefore, the critical diameter estimation based on the flow field in the absence of the particles becomes inaccurate as the critical diameter approaches that of the gap between the posts. Hence, for a given gap, the accuracy of the correlation for critical diameter will decrease for increasing critical diameters, that is, at large values of row-shift fraction ϵ .

III. EXPERIMENTAL VALIDATION

In this section, we present a detailed experimental validation of the universal correlation, Eq. (7), for the critical diameter of DLD arrays with polygonal posts. For experimental validation, we used the experimental data available in the literature and supplemented it with our own experimental data for conditions where published data were unavailable. For our experiments, we developed a novel approach to estimate the critical diameter by flowing droplets of varying diameter through the DLD array. To this end, we coupled a microfluidic droplet generator based on flow-focusing geometry, upstream of the DLD array. In contrast

to the typical experimental validation methods based on flowing particles and cells of fixed sizes, we could vary the droplet diameters over a wide range. This allowed us to precisely estimate the threshold between the zigzag and displacement modes of droplet migration. This section briefly discusses the design and fabrication of microfluidic devices with coupled droplet generator and DLD array, followed by the comparison of experimental data and theoretical correlation for critical diameter.

A. Device design and fabrication

The schematic of our experimental setup is shown in Fig. 7. Each DLD array with a different shape of posts was coupled with an upstream droplet generator based on the flow-focusing geometry. We used the flow-focusing droplet generator for two reasons. Firstly, varying continuous and dispersed phase flow rates can precisely tune the droplet diameter over a wide range. Secondly, in the flow-focusing droplet generator, the droplet generation is not affected by wall wettability as the continuous phase forms a lubricating film and prevents contact of the dispersed phase with the channel walls. For all the experiments, the designed width and height of the flow-focusing channels were 1000 μm each, except for the nozzle section. The height and width of the nozzle section were kept at 250 μm , and the nozzle length was 1000 μm . Different downstream DLD arrays were made with triangular, rotated square, and circular posts, each with a row shift fraction of 0.2.

The microfluidic devices were designed in CAD software (Autodesk Inventor), and the data was then converted into a rapid prototyping format (STL file). An open-source slicing software (CHITUBOX) was then used to slice the design into a series of thin layers. The processed data was transferred to a stereolithography 3D printer (ELEGOO Mars) based on the restricted surface method.²⁰ In the ELEGOO Mars setup, a UV laser beam with a wavelength of 405 nm was scanned over a liquid photopolymer epoxy resin (clear, Anycubic) to build the device layer by layer based on the sliced data. The three-dimensional features were fabricated with an accuracy of 50 μm . Finally, the microfluidic devices were thoroughly cleaned by flowing de-ionized (DI) water and isopropyl alcohol (IPA) through all the channels. Though similar dimensional accuracy can also be achieved using other microfabrication techniques, such as soft lithography, micro-milling, and laser ablation, stereolithography allowed the multilayered design of the droplet generator, where the nozzle is a square section

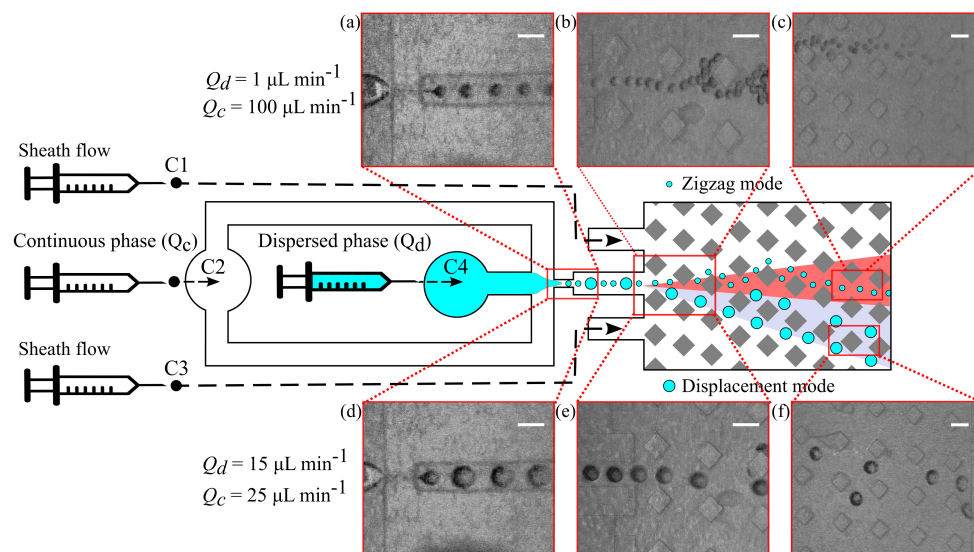


FIG. 7. Schematic of the experimental setup and microscope images demonstrating droplet generation and separation by size in the DLD device. The red and blue colored zones indicate the trajectories of droplets following zigzag and displacement modes, respectively. (a) and (d) show the generation of 250 μm and 720 μm droplets. The 250 μm diameter droplets flow in zigzag mode (b, c), and the 720 μm diameter droplets flow in displacement mode (e, f), and hence were collected by separate outlets. The scale bar represents 1 mm.

TABLE I. Measured geometric parameters of fabricated post shapes estimated at 95% confidence level. Dimensions were selected such that the critical diameter was similar for all polygonal posts.

Post shape	Post length (μm)	Gap (μm)	row shift fraction	Predicted critical diameter (μm)
Triangle	557 ± 5	1133 ± 5	0.20	530 ± 3
Square	791 ± 5	1129 ± 9	0.20	585 ± 5
Circle	605 ± 3	1000 ± 1	0.20	557 ± 1

at the center of the channel. The typical time for the fabrication process is 30 minutes.

Because of shrinkage and variability in the stereolithography process, the final device dimensions differed slightly from the designed dimensions. We used the measured dimensions of the fabricated devices to validate the correlation for critical diameter. Table I presents the measured geometric parameters of the fabricated DLD arrays, along with the critical diameter estimated from the correlation (Eq. (7)). The geometric parameters were chosen so that the critical diameter was comparable for all shapes, so that similar Q_d and Q_c could be used to validate the critical diameters. The random uncertainties in the measurements were estimated using t -distribution at a 95% confidence level. The geometric uncertainties were then propagated to the theoretical estimate of the critical diameter given by Eq. (7).²¹

B. Fluidic and optical setup

We conducted a total of 18 sets of experiments: five with triangular posts, six with rotated square posts, and seven with circular posts to validate the correlation given by Eq. (7). In our experiments, we used silicone oil (density $\rho_d = 950 \text{ kg m}^{-3}$, viscosity $\mu_d = 20 \text{ cSt}$, Sigma-Aldrich) as the dispersed phase and glycerol ($\mu_c = 1100 \text{ cSt}$, Sigma-Aldrich) as the continuous phase and the sheath fluid. For droplet generation, these liquids were infused into the device at varying flow rates using independent syringe pumps (KD Scientific, Legato 210). Droplet generation and trajectory in the DLD device were visualized using a stereo-zoom microscope (Radical Scientific, 6-45x zoom) equipped with a CMOS camera (Radical Scientific, Procam HS-5). The acquired images and videos were processed by subtracting the background image acquired only with the continuous phase in the device. Furthermore, we added a fraction of the background image without any fluid in the device to the processed image to show the location of the posts prominently.

For all the experiments, the droplet generation occurred in the dripping regime.²² In Fig. 7, we present the visualization of droplet generation and migration of droplets through the DLD array with square post. Figure 7(a) shows the generation of small droplets having a mean diameter of $250 \mu\text{m}$ when the flow rate of the dispersed phase was $Q_d = 1 \mu\text{L min}^{-1}$, and that of continuous phase was $Q_c = 100 \mu\text{L min}^{-1}$. These droplets flow through the DLD array in zigzag mode (Fig. 7(b)-(c)) as the droplet diameter of $250 \mu\text{m}$ is smaller than the critical diameter (predicted value $567 \mu\text{m}$). On the other hand, in Fig. 7(d) shows generations of larger droplets with a mean diameter of $720 \mu\text{m}$ for $Q_d = 15 \mu\text{L min}^{-1}$ and $Q_c = 25 \mu\text{L min}^{-1}$. Because the droplet diameter, in this case, is larger than the predicted $D_C = 585 \mu\text{m}$, the droplets flow in the displacement mode (Fig. 7(e)-(f)). For all the experiments, the sheath flow rate in the DLD device (as shown in Fig. 7) was kept constant at $500 \mu\text{L min}^{-1}$. Because of the high viscosity of the continuous phase (glycerol), the Reynolds number (computed based on the maximum velocity and array gap) was $\mathcal{O}(10^{-3})$.

We note that we observed no visible deformation of droplets with diameters up to $D_P/g \approx 0.5g$ as they migrated through the DLD array (see videos in the supplementary material). Consequently, their trajectory is expected to be the same as that of rigid particles. On the other hand, larger droplets ($D_P/g \approx 0.70 - 0.80$) were slightly deformed. Nonetheless, their hydrodynamic centre still lies outside the width of the first streamlane, making them

move in displacement mode. Also, the response time of the droplets to adapt to the spatial variation of the flow, $\tau_r = \rho_d D_P^2 / (18\mu_c)$ is $\mathcal{O}(10^{-6} \text{ s})$. This time scale is much smaller than the convective time scale given by, $\tau_c = g / u_{avg} \sim \mathcal{O}(1 \text{ s})$. Because $\tau_r \ll \tau_c$, the droplets quickly adapt to the spatial variations in the flow velocity. In the supplementary material, we show that the droplet trajectories in the experiments compare well with the computed streamlines.

C. Droplet generation and migration

Similarly, we performed droplet generation and migration experiments for varying flow rates of continuous phase (Q_c) and dispersed phase (Q_d) to accurately estimate the critical diameter of the DLD arrays. Figure 8 shows snapshots of droplet migration through the DLD array with square posts at varying flow rates of continuous and dispersed phases. As shown in Figs. 8(a)-(c), the 250, 375, and 550 μm droplets migrate in the zigzag mode. In contrast, larger droplets with diameters of 600, 720, and 780 μm (Figs. 8(d)-(f)), which were obtained at higher Q_d/Q_c ratios, undergo lateral displacement each time they interact with a post. Therefore, the larger droplets move in displacement mode. These experiments suggest that the critical diameter of this particular DLD array lies between 550 μm and 600 μm . As a comparison, the correlation, Eq. (7), predicts the critical diameter to be 585 μm , which is consistent with the experimental observation.

Similar to the experimental data shown in Fig. 8 for square posts, Fig. 9 shows snapshots of the droplet separation experiments with triangular posts. In Figs. 9(a)-(b), the 250 and 375 μm droplets migrate in the zigzag mode, and in Figs. 9(c)-(e), larger droplets with diameters of 550, 650, and 780 μm , undergo displacement mode. Therefore, the predicted critical diameter, $D_C = 530 \mu\text{m}$ with Eq. (7), agrees well with the experimental data.

As reported in the DLD literature⁹, we also observe that the transition from zigzag mode to displacement mode is not abrupt. Therefore, the performance of DLD devices is often quantified in terms of separation efficiency, defined as the ratio of particles/droplets separated into the targeted outlet to the total number of particles/droplets flowing through the device. In our experiments with triangular posts, the predicted critical diameter was 530 μm , and therefore, as expected, the separation efficiency for 550 μm droplets was relatively low (85.4%) compared with 99% efficiency for smaller and larger droplets.

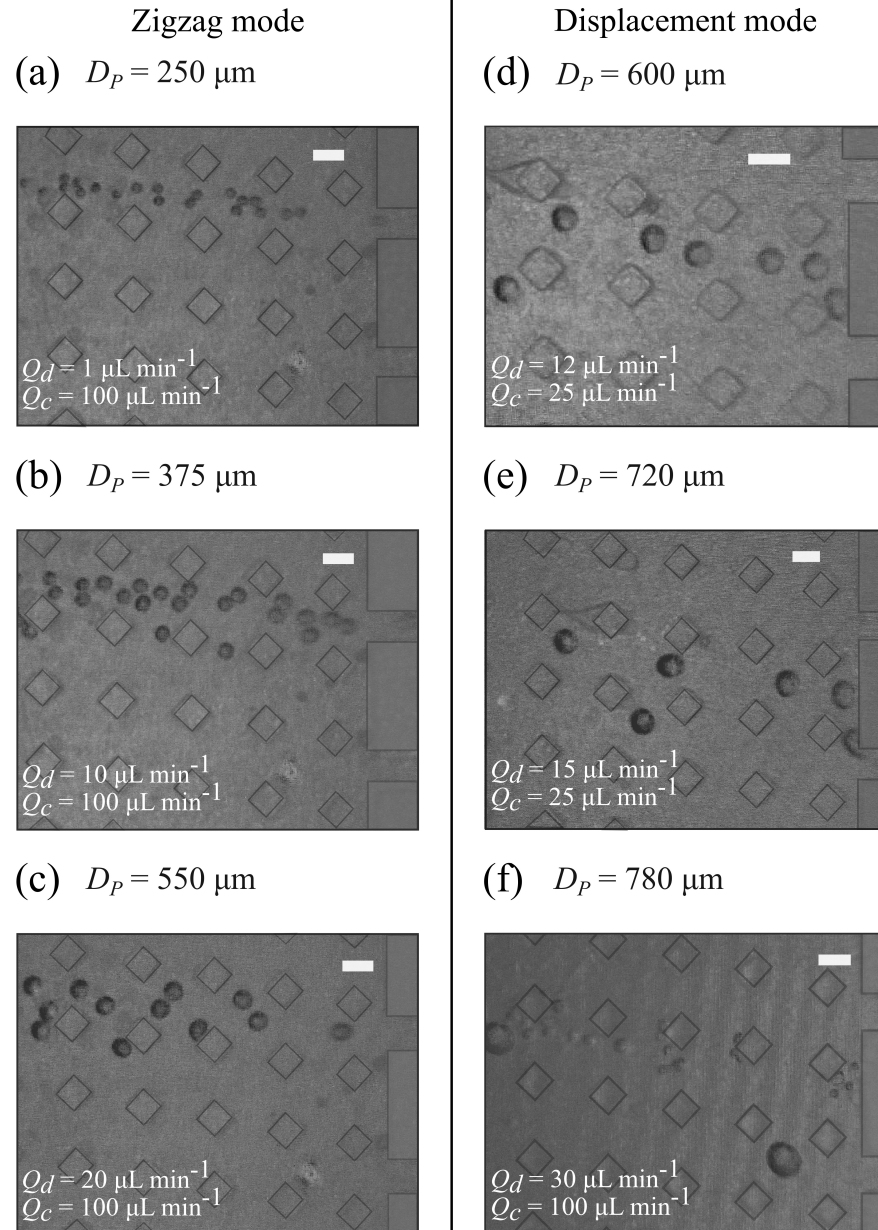


FIG. 8. Snapshots showing zigzag and displacement modes of droplets in DLD device with square posts. The DLD device was designed with row shift fraction, $\epsilon = 0.20$, gap, $g = 1129 \mu\text{m}$, for which the critical diameter predicted by Eq. (7) was $D_C = 585 \mu\text{m}$. The 250, 375, and 550 μm droplets travel in the zigzag mode, and the 600, 720, and 780 μm droplets migrate in the displacement mode. The scale bar represents 1 mm.

D. Experimental validation of the correlation

Similar to the experimental data shown in Fig. 8 for square post and in Fig. 9 for triangular post, we also performed droplet generation and migration experiments for DLD device with circular posts. In all, we performed experiments for 18 different conditions, including the

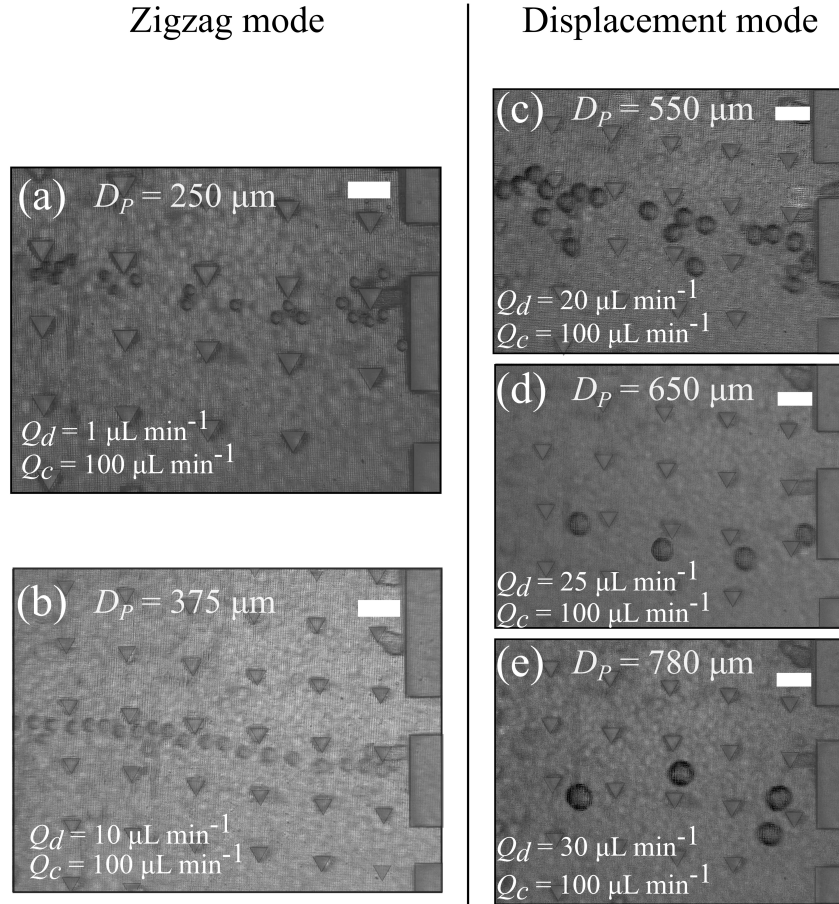


FIG. 9. Snapshots showing zigzag and displacement modes of droplets in DLD device with triangular posts. The DLD device was designed with row shift fraction, $\epsilon = 0.20$, gap, $g = 1133 \mu\text{m}$, for which the critical diameter predicted by Eq. (7) was $D_C = 530 \mu\text{m}$. The 250 and 375 μm droplets travel in the zigzag mode, and the 550, 650, and 780 μm droplets migrate in the displacement mode. The scale bar represents 1 mm.

post shape and flow rates of continuous and dispersed phases, while keeping the row shift fraction fixed at $\epsilon = 0.20$. In these experiments, the droplet diameters ranged from 220 μm to 730 μm . In addition, we used raw experimental data for 16 different conditions available in the literature^{9,14–17,23–30} to validate the correlation. We note that the critical diameter data available in the literature were primarily limited to circular posts (24 points). There were limited published data available for triangular (6 data points) and square (2 data points) posts, necessitating additional experiments.

Figure 10 presents the data from our and published experiments in a dimensionless form. In particular, in Figs. 10(a)-(c), we plot the dimensionless particle or droplet diameter D_P/g versus the row shift fraction (ϵ) for DLD arrays with triangular, square, and circular posts,

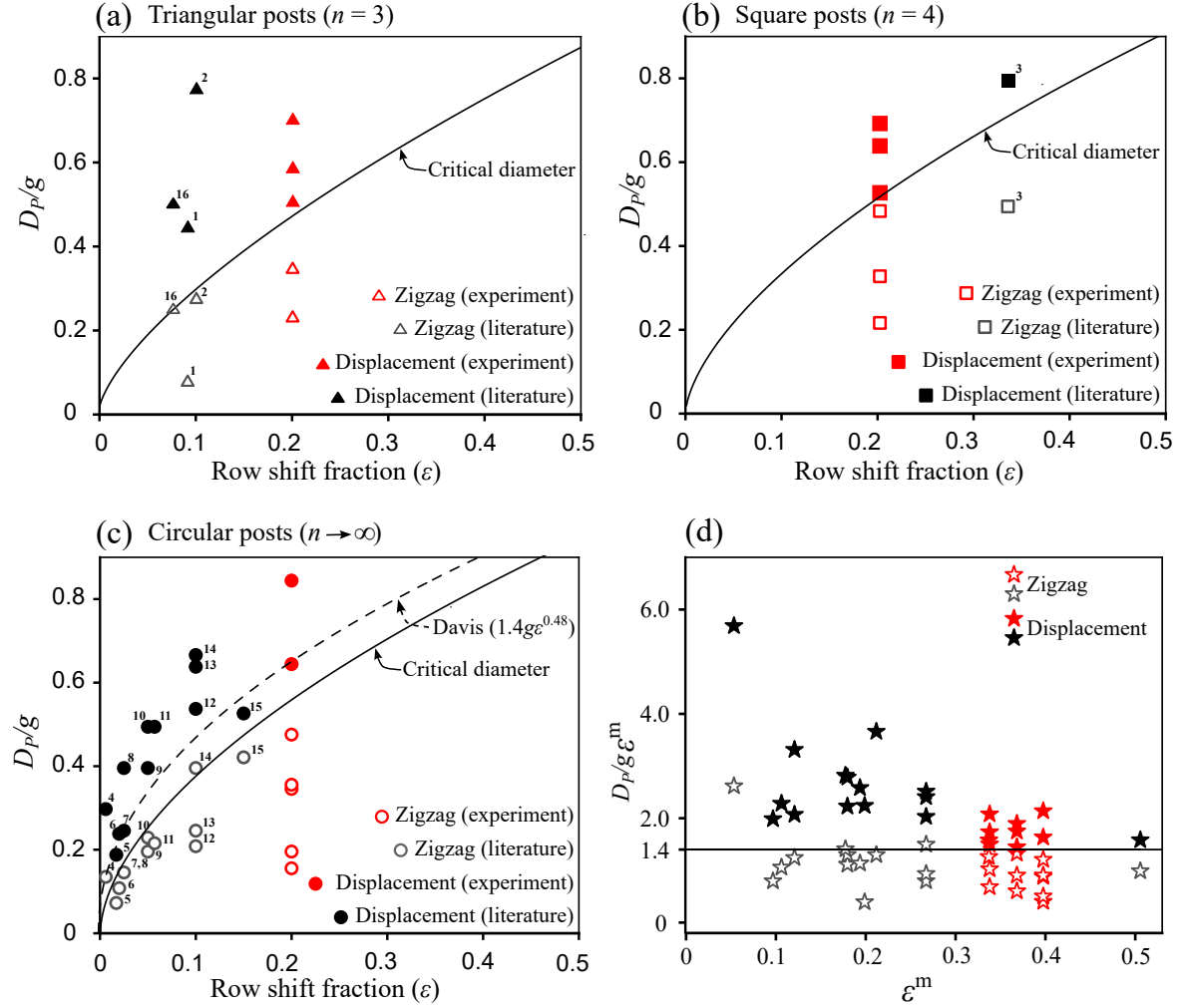


FIG. 10. Validation of the correlation with experimental data for (a) triangular, (b) square, and (c) circular posts. Solid points and open points represent displacement and zigzag modes, respectively. Black and red data points correspond to the experimental data from literature and our experiments, respectively. (c) also presents a comparison of our universal correlation with Davis's (Eq. (1)), showing better accuracy of our correlation at higher D_C/g ratios. (d) When all the experimental data is plotted on a $D_P/g\epsilon^m$ vs ϵ^m plot, the horizontal line at 1.4 separates most of the experimental data for displacement and zigzag modes. The experimental data points, numbered 1-15, are taken from the following works: (1) Louterback et al.,¹⁴ (2) Talha et al.,¹⁶ (3) Fandi et al.,¹⁵ (4) Inglis et al.,¹⁷ (5) Hattori et al.,²³ (6) Marhenke et al.,²⁴ (7, 8, 15) Nan Li et al.,²⁵ (9, 11) Inglis et al.,²⁶ (10) Zhang et al.,²⁷ (12) Wunsch et al.,²⁸ (13) Huang et al.,⁹ (14) Green et al.,²⁹ and (16) Pariset et al.³⁰.

and compare them with the critical diameter predicted by Eq. (7). In Fig. 10, solid symbols correspond to particles or droplets that migrate in the displacement mode through the DLD array, whereas hollow symbols correspond to the zigzag mode. Figures 10(a)-(c) show that the theoretical correlation, Eq. (7), correctly classifies zigzag and displacement modes of particle migration through the DLD array based on the critical diameter. Moreover,

our experimental data using droplets is consistent with published DLD experiments with particles, suggesting that our approach can be reliably used for experimentally estimating critical diameter of DLD array. We have also plotted the correlation given by Davis (Eq. (1)) in Fig. 10(c). Our universal correlation demonstrates better accuracy at higher D_C/g ratios compared to Davis's correlation. This enhanced accuracy can be attributed to our correlation being derived from an extensive set of simulations, whereas the correlation proposed by Davis et al. was developed based on a limited experimental dataset.

Finally, in Fig. 10(d), we replot all the experimental data with $D_P/g\epsilon^m$ on the ordinate and ϵ^m as the abscissa. We observe that a horizontal line at 1.4 separates most of the experimental data for displacement and zigzag modes. This shows that the correlation given by Eq. (7) can accurately predict the critical diameter of DLD arrays with polygonal posts.

Overall, the correlation Eq. (7) based on the simulations predicts, and our experiments validate, the following: Firstly, for a given post-shape, the critical diameter increases with an increase in the row shift fraction or decrease in the periodicity n of the DLD array. Secondly, the critical diameter scales proportionally with the gap between the posts. Finally, the critical diameter decreases with the number of sides of the polygonal post, with differing rates for even and odd-sided polygons.

IV. CONCLUSION

We presented an experimentally validated correlation to estimate the critical diameter of DLD arrays with polygonal posts based on geometric parameters including the shape of the posts, the gap between the posts, and the relative shift between the adjacent rows of posts. The correlation was developed based on a large set of simulations of fluid flow in DLD arrays with triangular, square, pentagonal, square, hexagonal, heptagonal, octagonal, and circular posts. To validate the correlation, we used a novel experimental approach of coupling a DLD array with an upstream droplet generator to perform DLD experiments with droplets of varying sizes in arrays with triangular, square, and circular posts. We supplemented our experimental data with experimental data available in the literature. Our universal correlation correctly classifies the zigzag and displacement modes observed in our experiments as well as in those reported in the literature.

A typical DLD device design may require conflicting constraints. For example, reducing the gap between the posts to decrease the critical diameter may lead to clogging of the device. On the other hand, a lower row shift fraction or higher periodicity to obtain smaller critical diameter results in a longer device. The post shape may also be constrained by the fabrication method. The experimentally validated correlation for critical diameter presented here can be used for optimization of DLD devices to achieve a desired critical diameter under various constraints on the design parameters.

V. SUPPLEMENTARY MATERIAL

The supplementary material contains the following additional information:

1. The details of the boundary conditions used in the simulations.
2. A comparison of 2D and 3D simulations.
3. The effect of post size on the critical diameter.
4. A comparison of droplet trajectories in experiments with simulated streamlines.
5. Discussion on droplet deformation in the DLD devices.

ACKNOWLEDGMENTS

We acknowledge the financial support received from the Science and Engineering Research Board (SERB), Government of India, under the Core Research Grant scheme (Grant No. CRG/2022/002148) and the Mathematical Research Impact Centric Support (MATRICS) scheme (Grant No. MTR/2022/000080). The authors have no conflicts to disclose.

CONFLICTS OF INTEREST

There are no conflicts to declare.

DATA AVAILABILITY

The data that supports the findings of this study are available within the article.

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PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0214178

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