Simulation and experiment of capillary-driven planar baffle micromixers

Chen-Kuei Chung, B.T. Liang, C.C. Lai

Department of Mechanical Engineering and Center for Micro/Nano Science and Technology, National Cheng Kung University, Tainan, Taiwan
E-mail: ckchung@mail.ncku.edu.tw

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Different capillary-driven planar baffle micromixers with a trigger valve which were fabricated on polymethylmethacrylate sheets using CO_2 laser ablation and thermal bonding are investigated. Two main modified staggered and meander baffle structures were used to compare the mixing efficiency. The modified staggered baffle structure has lower capillary flow resistance and faster speed compared with the meander one. Conversely, the meander baffle structure has higher mixing efficiency at lower flow speed with enough diffusion time than the modified staggered one. The effective channel height of the trigger valve was simulated to be between 220 and 434 µm for merging two fluids at negative capillary pressure. The experiments also verified the trigger value worked at the channel height of 351 µm for two fluids merged together to flow forward but it failed at 169 µm height for only one fluid flow without merging. The mixer with the meander baffle structure performed wiht the best mixing efficiency of 94% among the design structures because of the long flow time and short average diffusion length in the mixing zone.

1. Introduction: Microfluidic mixing plays a crucial role in applications relating to biological, medical and chemical synthesis and analysis devices at low cost. Good mixing creates good interdiffusion and reactions between the sample and the reagent. Generally, two types of micromixer, i.e. active and passive ones, have been developed [1–3]. Active mixers introduce external energy such as magnetic force [4], the thermal gas bubble [5] or the active channel switch [6] to disturb the flow field for mixing enhancement within microchannels. Passive mixers include specific channel geometries to induce chaos advection and lamination without external energy such as the splitting/recombination channel structure to increase the diffusion effect for mixing enhancement [7]. In simple comparison, active mixers perform better mixing than passive mixers, but the presence of the external energy source and its components brings about problems in chip integration, reliability and other side-effects. The passive micromixer in three-dimensional (3D) structures requires more complicated fabrications such as multi-step lithography or multiple layers alignment [8, 9]. This is unfavourable to low-cost chip fabrication and integration but can be overcome by the 2D planar micromixer [10, 11]. Besides, the above micromixers generally need a fluid pumping system including a syringe pump, tubes and a power supply which is not suitable for non-technical users without basic training. Therefore, a feasible way is to apply a capillary-driven system with fine design for ease of operation. For capillary flow at a low Reynolds number (Re < 2), the molecular diffusion mechanism dominates the micorfluidic laminar flow. The diffusion time is proportional to L^2/D where L is the diffusion length, and D is the diffusion coefficient. A long length of time and a long channel length are required for complete mixing at low Re. Therefore, a good capillary passive micromixer is designed to effectively reduce mixing time and channel length.

In the work reported in this Letter, four 2D baffle micromixers, i.e. staggered, modified staggered, modified paralled and meander baffle structures, with a capillary trigger valve, were designed to determine an efficient micromixer. The modified staggered and meander baffle structures are compared by simulation and experiment for mixing efficiency and average Re after the effective capillary trigger valve. The 2D numerical simulations were carried out to examine the trigger mechanism and mixing efficiency.

2. Simulation and experimental procedures: Fig. 1 shows the design of one schematic baffle mixer consisting of two inlets for two mixing fluids and a trigger valve structure to ensure the two fluids arrive at the inlet of the mixing unit. After the trigger valve, there are 15 repeated baffle type mixing units 18 mm long. The outlet channel is 7 mm long to ensure that the flow line is laminar, and that the flow speed is slow enough for observation. The capillary pressure is applied and four different baffle structures (staggered, modified staggered, modified parallel baffle structure, meander baffle structure) with a capillary trigger valve are analysed, to find out the effective channel height by simulation.

The commercial fluid multiphysics simulation software (CFD-ACE) was used for studying the trigger valve and mixing performance. The model was designed by AutoCAD and imported to the software which assumed no fluid slip along the channel wall, Newtonian fluid and no compressible surface tension. After all the fluid properties (water) and boundary conditions (air) were set, the model was mashed as a square with the element number of 14 720. The mixing index (M) is calculated by the following equations

$$M = 1 - \frac{\sigma}{\sigma_{\max}} \tag{1}$$

and

$$\sigma = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(c_i - \bar{c})^2} \tag{2}$$

where n is the amount of the sample, σ is the standard deviation of the concentration, $\sigma_{\max}$ is the maximum deviation of the concentration, c_i is the concentration of each sample point, and $\bar{c}$ is the average concentration. $M = 0$ (0%) represents no mixing effect, $M = 1$ (100%) is for complete mixing and $M \geq 0.9$ is considered a good enough mixing. The mixing index is calculated by the image analysis of the colour intensity captured by a CCD camera.

The mixer chips were made of polymethylmethacrylate (PMMA) plate (2 mm thick with a contact angle of 68°) by CO_2 laser ablation. The commercial air-cooling CO_2 laser equipment (VL-200, Universal Laser System Inc., USA) with a maximum laser power of 30 W was used. The CO_2 laser has a wavelength of 10.6 µm

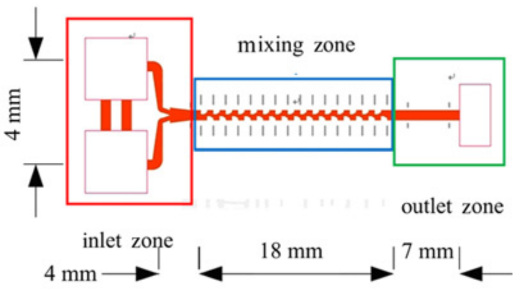

Figure 1 *Micromixer design with inlet zone (red), mixing zone (blue) and outlet zone (green). The relative dimensions are given in Section 2*

and the maximum laser scanning speed of 1140 mm/s. After several tests for trigger valve function, the PMMA was finally fabricated at a 5 W laser power and an 11.4 mm/s scanning speed 100 times for the channel and trigger valve with the depth of about 351 µm and another 100 times for the inlets. Then the laser ablated PMMA plate was cleaned by ultrasonic cleaner and thermally bonded with the flat PMMA plate. The mixing experiments were carried out by mixing light red and blue dyes and observed with the CCD camera on an optical microscope (OM, OLYMPUS BX51M, Japan). The channel profile was observed with an α-step profiler (Kosaka Laboratory, ET3000, Japan) [12].

3. Results and discussion: Fig. 2 shows the four structures of the mixing channel design. The repeated unit has an overall channel width of 1 mm and length of 1.2 mm.

Fig. 2*a* is the staggered baffle structure with the mixing block length of 0.6 mm and block width of 0.4 mm with a serial of broadening and narrowing the channel. Fig. 2*b* is the modified staggered baffle structure, with a block length of 0.6 mm and a block width of 0.4 mm at a 30° titling angle which is designed to reduce the flow resistant and increase the flow stability. Fig. 2*c* is the modified paralled baffle structure, with a block length of 0.6 mm and a block width of 0.2–1 mm at a 30° titling angle with a serial of broadening and narrowing the channel. Fig. 2*d* is the meander baffle structure, with the block height increased to 0.7 mm and the block width reduced to 0.3 mm for a longer flow channel and a low diffusion length to enhance the diffusion effect. As the capillary flows, a slight vortex follows as a result of the geometry change of the channel which enhances the diffusion effect by the large chance of the interaction of the fluid. By capillary analysis, we can find out the effective channel design region to avoid flow problems such as bubble clog or self-clog. It indicates that modifying the baffle structure with corner cutting can increase the effective channel height design region. However, the staggered baffle structure has sharp corners which can increase the flow resistance by alternate changes of channel width as well as the unstable capillary pumping force due to the frequent change of the contact angle at the front end of the fluid flow. So the modified staggered baffle structure reduces the capillary resist together with diffusion length by trimming the sharp angle. The modified paralled baffle structure can also reduce the diffusion length by double tilting the channel, however the capillary flow resist will increase greatly as a result of the increase in block width. The meander baffle channel is the better channel design for capillary pumping with small change in contact angle and better mixing for the efficient reduction of the diffusion length. We tested the design and finally used both the modified staggered baffle and meander structures for further comparison of flow and mixing behaviour.

The effective channel height of the trigger valve can be simulated by capillary pressure of the valve microstructure. It suggests that the trigger valve height with the normal function is between 220 and 434 µm as the capillary pressure is negative at the duration of before and after merging, respectively. Two channel heights of 169 and 351 µm were used in the experiments to verify the effective channel height region of the trigger valve in the straight channel as shown in Fig. 3. The meniscus flow cannot stop in the junction of the trigger valve at the channel height of 169 µm and gets bubble stuck always due to positive capillary pressure, so only single fluid flows ahead and fails the trigger effect (Figs. 3*a* and *b*). In contrast, the trigger valve functions normally at the channel height of 351 µm as one meniscus flow gets stuck because of negative capillary pressure in the locally narrowest place to wait for another fluid's arrival to merge together and forward (Figs. 3*c* and *d*).

Figs. 4*a* and *b* show the simulate mixing index after the triggering valve by the flow time at different diffusion coefficients (D) of 10^{-8} m^2/s and 10^{-10} m^2/s, respectively. The different mixing index is due to the capillary pumping and the diffusion effect of the fluid within the microchannel. So in 1.76 s after the triggering valve, the mixing happens in the simulation, and the actual experiment time has to add the triggering valve delay time. The larger mixing coefficient of 10^{-8} m^2/s will result in better mixing effect and quick mixing within the short time. However, the mixing efficiency is a fast trend to achieve good mixing (>90%) within the fluid flow at 1–2 s. If D is 10^{-10} m^2/s, the mixing efficiency is linear compared with $D = 10^{-8}$ m^2/s, but it is more reasonable in the normal condition owing to absence of overshoot situation. The fluid used for mixing is water with a diffusion coefficient of 2.32×10^{-9} m^2/s between both 10^{-8} and 10^{-10} m^2/s. So it is helpful to simulate

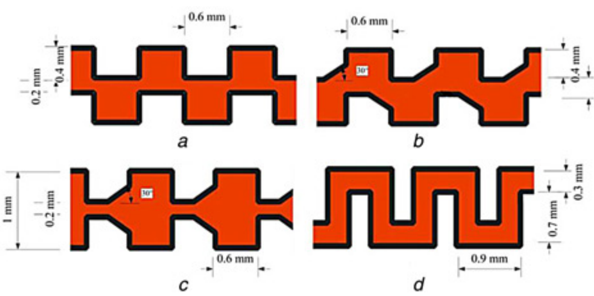

Figure 2 *Four structures of the mixing microchannel*
a Staggered baffle
b Modified staggered baffle
c Modified paralled baffle
d Meander baffle

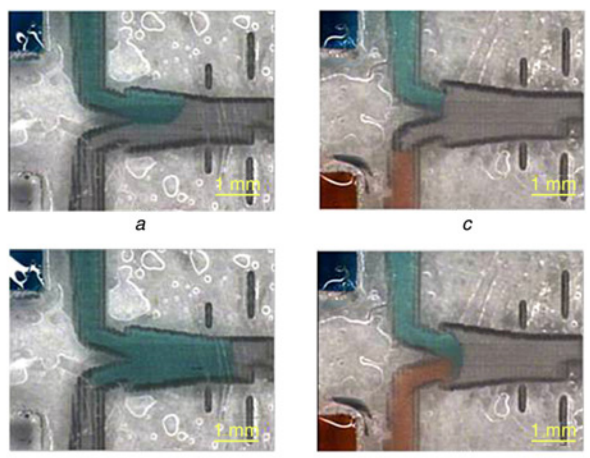

Figure 3 *Test for trigger valve function at a channel depth of 169 µm at t = 2 s (Fig. 3a) and t = 4 s (Fig. 3b) (trigger fails); and at a channel depth of 351 µm at t = 2 s (Fig. 3c) and t = 4 s (Fig. 3d) (trigger works)*

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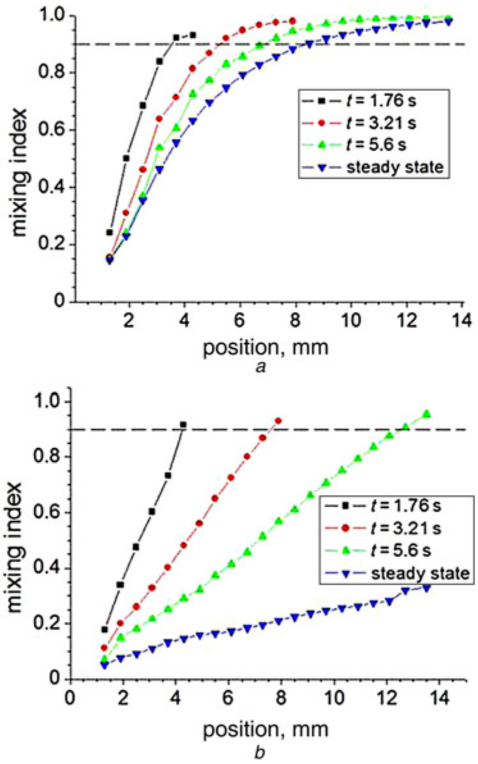

Figure 4 *Mixing efficiency at diffusion coefficient $D = 10^{-8}$ m^2/s (Fig. 4a) and $D = 10^{-10}$ m^2/s (Fig. 4b)*

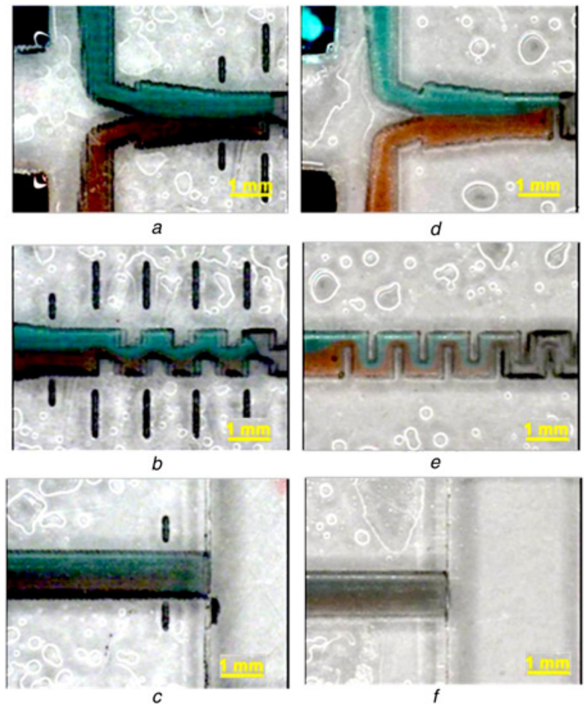

Figure 6 *Comparison of mixing behaviour between the modified stagger baffle channel at various times: t = 2 s (Fig. 6a), t = 7 s (Fig. 6b), and t = 40 s (Fig. 6c); and the meander baffle channel at various times: t = 2 s (Fig. 6d) t = 16 s (Fig. 6e), and t = 71 s (Fig. 6f)*

and compare the results with a diffusion coefficient between 10^{-8} and 10^{-10} m^2/s.

Figs. 5*a* and *b* show the actually merged microscope photos of the mixing test in both structures of the modified staggered baffle and meander baffle structure with the trigger valve, respectively. The sample consists of two inlets and is followed by the trigger valve with a distance of 4 mm for two fluids to merge together and forward. The detailed experiment results for the comparison of both structures are shown in Fig. 6.

Fig. 6 shows the comparison of mixing behaviour between the modified staggered baffle channel and the meander baffle channel. Both dilute blue and red dyes are filled in each inlet. The two colour dyes start to flow towards the trigger valve by the capillary force. The trigger valve delays one dye until the other arrives to release the first dye then they flow together to mix forward. At $t = 2$ s, the two colour dyes meet and flow together in both the modified staggered and meander baffle channels by the trigger valve effect (Figs. 6*a* and *d*). The two fluids in the modified staggered structure arrive at the fourth mixing unit at 7 s and the flow speed is slowed down together with the mixing occurrence (Fig. 6*b*). The fluids in the meander channel take a longer time of 16 s to arrive at the same position of the fourth mixing unit (Fig. 6*e*). It shows that the flow speed of the meander channel is much slower than that of the modified staggered baffle channel due to larger flow resistance. The mixed fluids in the modified staggered structure arrive at the outlet at 40 s (Fig. 6*c*) while it takes 71 s to for a flow through the meander channel along with as better mixing (Fig. 6*f*).

Table 1 summarises the flow and mixing test results for the trigger valve, together with the modified staggered and meander baffle structures at the channel height of 351 μm. The straight channel with only the trigger valve only takes <10 s total flow time and the average Re is <1.48 for the mixing efficiency of only 53%. The staggered baffle structure has bobble clogging and cannot complete the flow. The modified staggered baffle structure takes 40 s to flow through the whole channel and the average Re is 0.32 for a mixing efficiency of 63%. The modified paralled

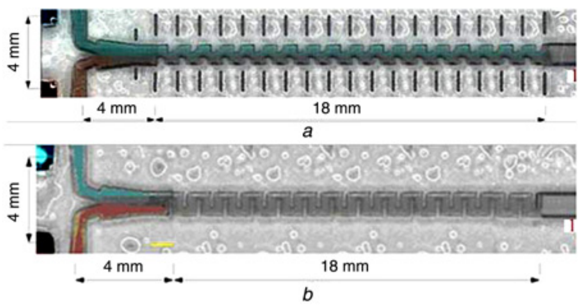

Figure 5 *Actually merged microscope photographs of mixing test of both structures in the modified staggered baffle structure at* t = *40 s (Fig. 5a) and the meander baffle structure at* t = *2 s (Fig. 5b)*

Table 1 Results of flow and mixing test for trigger valve, together with the modified staggered and meander baffle structures at channel height of 351 μm

Pattern	Flow test		Mixing test
	Total flow time, s	Average Re	Mixing efficiency, % at $t = 80$ s
only trigger valve	<10	<1.48	53
modified staggered baffle structure	40	0.32	63
meander baffle structure	71	0.18	94

baffle structure has larger vibration of the capillary pumping force and bobble clogging so as not to complete the flow. The meander baffle structure with the slowest flow takes 71 s to flow through and the average Re is 0.18 for the highest mixing efficiency of 94%. The modified staggered baffle structure has a fast flow speed but low mixing efficiency while the meander baffle structure has a slow flow speed and good mixing efficiency. Moreover, the Re in all the baffle mixers is very low (<0.5) and strongly suppress as a vortex pair in the meniscus. Mixing enhancement is mainly contributed from nature diffusion related to diffusion length and time. Therefore, the meander structure performs with the best mixing efficiency due to the shortest diffusion distance and longest diffusion time.

4. Conclusion: We have successfully investigated capillary-driven planar baffle micromixers with a trigger valve made of laser ablated PMMA. Four kinds of structures including the staggered, modified staggered, modified paralled and meander baffle structures were designed for comparison of flow and mixing behaviour. The structure geometry consists of the trigger valve, 15 mixing units at a total of 18 mm length and at an outlet 7 mm long. The staggered baffle and modified paralled baffle structures are skipped for the clogging problem and low capillary pumping. By the simulation, the effective channel height of trigger valve is between 220 and 434 μm as the capillary pressure is negative at the duration of before and after merging of the two fluids. The 351 μm depth was selected for the experiments. In the flow test, the modified staggered structure had a faster flow speed to complete the full channel flow within 40 s but a low mixing efficiency of 63% compared with the meander baffle structure with a longer flow time of 71 s and a better mixing efficiency of 94%. In brief, the diffusion dominates the mixing behaviour of the capillary-driven baffle micromixer. The meander baffle structure performs best because of the longest mixing time and the shortest average diffusion distance.

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