Abstract

This paper presents a micro flow discretizer that digitizes continuous liquid flow into nanoliter segments. To study the interfacial forces and facilitate the device implementation, numerical simulations are performed and the results are used to guide the design process. In the prototype demonstration, the discretizer is made of Polydimethylsiloxane (PDMS) microfluidic channels with desired geometry and surface properties. With the assistance of a pair of externally applied and independently controlled pressures, a continuous water flow has been split into segments with controllable volumes. As such, this flow discretizer opens up a new class of metering and manipulation scheme in microfluidic applications such as lab-on-a-chip and drug discovery.

1 Introduction

Separation of liquid segments from a continuous source has been studied for decades. For example, a growing pendent drop may break away under gravity (as shown in Fig. 1) once it can no longer be supported by surface tension [1-3]. When dimensions shrink, breakaway becomes more difficult because of stronger surface effects at the microscale. Micro droplets with sizes ranging from a few to hundreds of micrometers have numerous applications in various areas, such as inkjet printing, fuel injection, miniature optical systems, IC cooling, combinatorial chemistry, bioassays, and drug delivery [4]. Previously, researchers had demonstrated micro droplet separation by using many different approaches, including electro-wetting-on-dielectric (EWOD) schemes [5, 6], thermal bubble [7, 8], PZT [9, 10], or pressurized air actuation [11]. Furthermore, in a system containing two immiscible fluids mixed with a surfactant, liquid droplets of one fluid can be generated and dispensed in the continuous phase of the other liquid [12-14]. To achieve droplet separation, all these approaches require sophisticated control. However, most of these approaches can only generate droplets with fixed and pre-determined volumes.

This work presents a new separation scheme by the assistance of desired channel geometry and externally applied pressures to realize variable flow discretization for lab-on-a-chip applications. Three accomplishments have been achieved: (1) design rules verified by both numerical simulations and experimental results to facilitate the device implementation; (2) a simple fabrication process employing molding and bonding schemes to construct microfluidic networks on polymeric substrates; and (3) a variable flow discretizer with minimum control. As such, this scheme can be integrated with bioassay or lab-on-a-chip systems to provide metering and manipulating functions of fluidic samples, buffers, or drugs.
2 Principles and Theoretical Models

Surface tension is referred to as a free energy per unit area, or may equally well be thought of as a force per unit area [15]. When a droplet is separated from a continuous source, work is done by the applied forces against the interfacial tension to discretize the droplet, thereby creating additional surface area between liquid and air (or between liquid and the another liquid) while conserving the total liquid volume. Therefore, a net energy is added into the system and stored on the interfaces as the form of surface free energy. Furthermore, the applied forces must be arranged in an appropriate configuration to interact with the interfacial forces. There are a variety of sophisticated approaches that can accomplish this. In this work, we focus on an approach that employs two pressure sources to discretize a continuous flow into micro droplets in closed microfluidic channel. In this scheme, we need one positive pressure applied upstream and a negative pressure applied downstream. These two pressures are arranged to act in the same direction but driving the liquid with different flow rates. The difference in flow rates eventually causes the discretization with the assistance of air supply from the ambience. Fig. 2 shows the operation principle: (a) a steady and continuous flow is driven by a positive pressure in a hydrophobic microfluidic channel and moves into a junction area; (b) flow reaches the entrance on the other side of the junction, where a negative pressure is applied to suck the flow front into the channel downstream; (c) since the flow rate caused by the negative pressure is higher than the flow rate caused by the positive pressure upstream, the front part of the flow and certain volume of air, which flows at a rate equal to the difference of flow rate caused by the negative and positive pressures, are sucked into the small channel downstream; (d) finally, the process completes and a droplet is generated and driven forward in the microfluidic channel downstream. This concept is straight-forward and can be easily implemented on a microfluidic chip. Fig. 3 shows the schematic design of the proof-of-concept prototype. The inlet inter-connection supplies the incoming liquid, the two air vents are designed to supply air while assisting the separation process, and the outlet is connected to a vacuum source to provide the negative pressure downstream.

\[
\Delta P = \frac{2\gamma \sin \theta}{w}
\]  

where \(\gamma\) is the surface energy of gas/liquid interface, \(w\) is the width of the microfluidic channel, and \(\theta\) is the contact angle of the channel surface. In Fig. 4(a), the pressure required to push the working flow moving
downstream will drop when the flow reaches the junction. While the working liquid is driven into the small hydrophobic channel downstream, additional pressure is required as shown in Fig. 4(b). The required extra pressure to assist the separation of the flow will be provided by the vacuum source downstream.

![Pressure barriers built across the junction](image)

Fig. 4: Pressure barriers built across the junction

![Schematic diagram of the basic element used in the simulation program for surface energy minimization](image)

Fig. 5: Schematic diagram of the basic element used in the simulation program for surface energy minimization

The most critical step in the splitting sequence is the final breakaway process. Overcoming the pressure barriers built across the junction doesn’t necessarily provide enough forces to break the flow. To have a better understanding and to identify critical parameters related to the splitting of flow, a simulation program, Surface Evolver [16], is employed. First, an initial shape is applied and the constraints that surfaces should satisfy are also defined. Energy functions associated with three-dimensional surfaces are specified afterward. Surface Evolver then discretizes the surfaces into small triangular elements and modifies these elements, subject to the given constraints, to minimize the overall surface energy. Considering an individual triangular element, as shown in Fig. 5, its surface energy can be expressed as:

\[ E = \frac{T}{2} \| \mathbf{V} \times \mathbf{S} \| \]  

(2)

where \( T \) is the surface energy per unit area and \( \mathbf{V}_0 \) and \( \mathbf{V}_1 \) are two edge vectors of the element. Since the derivative of strain energy with respect to displacement equals the corresponding force, the surface tension force induced at one specific vertex can be expressed as:

\[ \mathbf{F}(\mathbf{V}_0) = \frac{T}{2} \frac{\mathbf{V}_0 \times (\mathbf{S}_0 \times \mathbf{S}_1)}{\| \mathbf{S}_0 \times \mathbf{S}_1 \|} \]  

(3)

![A successful breakaway sequence simulated by Surface Evolver](image)

Fig. 6: A successful breakaway sequence simulated by Surface Evolver

By moving each vertex along the net force induced at it, the overall surface energy will eventually reach its minimum and the equilibrium state can be found. In the current case, the overall energy is the sum of surface energy corresponding to its free surfaces and its contact energy with the channel walls. Fig. 6 shows an evolving sequence that predicts a successful breakaway in the microfluidic channel. In this case, the junction length \( h \) is long enough to cause the surface to become unstable and breakaway will naturally occur to minimize the overall surface energy. The depth \( d \), widths \( w \), and length \( h \) of the hydrophobic microfluidic channel are identified as the critical parameters and numerical simulations are performed to characterize the criteria of natural breakaway.
3 Fabrication Process

Polydimethylsiloxane (PDMS) is used to fabricate the device for demonstration and the fabrication process is shown in Fig. 7 [17, 18]. First, a layer of 50 µm thick negative photo-resist (MicroChem SU-8) is spin-coated and patterned on top of a clean silicon wafer to create a mold for duplicating microfluidic components in the following polymer casting process. After the SU-8 mold is fully cured, it is coated with a thin layer of Teflon to reduce the adhesion and to facilitate the removal of the polymeric replica after casting. A mixture of 10:1 PDMS pre-polymer and curing agent (Dow-Corning Sylgard 184) is stirred thoroughly and then degassed under vacuum. The pre-polymer and curing agent mixture is then poured onto the mold, degassed, and cured for 2 hours at 80°C. In this work, the PDMS replica is 5 mm thick to keep the device mechanically stable during the connection and operation processes. Once cured, this PDMS replica is peeled off from the mold and punched to construct holes for inter-connection. On the other hand, another PDMS layer made of a 30:1 mixture is cast with a thickness of 2 mm. These two layers are then brought into intimate contact and cured for another 2 hours at 85°C to achieve irreversible bonding. Finally, Teflon and silicone tubes are inserted to make inter-connection to external pressure sources.

4 Measurement Results and Discussions

Fig. 8 shows a complete sequence of the discretization process that concurs with the operation principles shown in Fig. 2. The dimensions of the microfluidic channel are specified following the rules acquired from the simulation results to ensure successful breakaway. The volumes of the discretized segments are measured to be ranging from 10 to 30 nanoliters controlled by the channel geometry and the pressure applied across the junction. The breakaway process takes less than 1 second to complete and is controlled by the incoming and outgoing flow rates. The volume of discretized segment is determined by the dimension of channel, especially the width (w) of the channel and the length (h) of the junction as indicated in Fig. 6. The depth will also affect the results but currently all the experiments used microfluidic channels with a fixed depth of 50 µm. Because of the low elastic modulus of PDMS, volume variation caused by channel deformation is also observed.
For practical applications, this flow discretizer can be integrated with other bioassay or lab-on-a-chip systems to provide metering and manipulating functions of fluidic samples, buffers, or drugs.

5 Conclusions

A micro flow discretizer that digitizes continuous liquid flow into nanoliter segments is demonstrated. The prototype discretizer is made of PDMS with simulation-verified geometry and surface properties for flow separation. The operation principle of the flow separation is based on the design of geometry and surface property to control the separation of flow at the microscale. With the assistance of channel geometry and external pressure sources, successful discretization of continuous water flow into segments with volumes from 10 to 30 nanoliters has been demonstrated. Future work may include the integration with other microfluidic devices to construct a complete system. As such, this autonomous flow discretizer represents a new class of metering and manipulation scheme for applications including lab-on-a-chip and drug delivery systems.

References