Modeling of Multi-Phase Flows in MEMS World

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1. MEMS and Simulation Based Design

MEMS is acronym for Micro-Electro-Mechanical System, or mechanical integrated circuits. It represents a fast growing new technology that fabricates micro-devices using processes similar to those used in the Integrated Circuit industry. These micro-devices are physically small (on a scale of microns to millimeters) and often have both electrical and mechanical components on the same chip. They have two vital advantages over conventional counterparts. First, they are usually batch fabricated, so hundreds to thousands can be manufactured at once, which makes them potentially cheap and plentiful. Secondly, these micro-devices can be directly integrated with integrated circuits, hence the costs of assembly are greatly reduced and far more complicated systems can be made than with any other technologies.

Quantitative design plays a key role in MEMS. It permits prediction of performance prior to building a device, supports the troubleshooting of device designs during development, and enables critical evaluations of failure mechanisms after device has entered manufacturing.[1-1]. This in turn further requires an in-depth understanding of the operating characteristics of such devices necessary for component design and system integration. Numerical simulation provides quantitative analysis of different aspects of devices, and significant insight across multi-disciplines such as electronics, mechanics, chemistry, thermal science and fluid science [1-7] that is present in the components. Simulation based design is gaining acceptance amongst MEMS researchers and engineers and is regarded as means not only to interpret experimental data [1-4] but also to explore the entire parameter space that influences the performance of a device, which is relatively hard experimentally. Simulation-based design analysis "can avoid costly, iterative experimental design process where components are fabricated, tested, and then redesigned to improve performance" [1-5][1-6]. **Application of *DropSim*^{TM}*/BubbleSim*^{TM} to simulation based MEMS design is the theme of this paper.**

The first commercial MEMS application emerged twenty-five years ago in form of pressure sensors initially supporting aerospace. Now the MEMS market consists of segments of optical, biotech, displays, RF & ICs, sensors and actuators, etc. with $2.5 Billion sales in year 2000 [1-2]. "Successful stories" include pressure sensors, accelerometers, projection displays, ink jet nozzles, bio-chips, fiber optic switches, etc. [1-3]. In this paper we will demonstrate ***DropSim***^{TM}***/BubbleSim***^{TM} as a state-of-art multi-phase flow simulator with MEMS design applications across almost all MEMS market segments especially ink-jets and bio-tech areas.

Reference

[1-1] Senturia, S. D., Microsystem Design, Kluwer Academic Publishers, 2001
[1-2] Bryzek, J., The 11th International Conference on Solid-State Sensors and Actuators, Munich Germany, June 2001
[1-3] Petersen, K. E., Solid-State Sensor and Actuator Workshop, Hilton Head Island, South Carolina, June 2000
[1-4] Hsing, I.-M., et al, Chem. Eng. Sci., 55, 1
[1-5] Jensen, K. F., Solid-State Sensor and Actuator Workshop, Hilton Head Island, South Carolina, June 2000
[1-6] Zeng, J., et al, Micro-Electro-Mechanical Systems 2000, American Society of Mechanical Engineers, Vol. 2, pp.581-587
[1-7] Zeng, J., et al, Proceedings of 6th Annual Conference of Micro-Electro-Mechanical Systems Technologies, State Commission of Micro-Electro-Mechanical Systems Technologies, R.O.C.

2. *Design Applications I: Ink-Jet Printing Head*

Despite the belief that we have been supposedly moving toward the "paperless" world for 30 years, the market is still starving for simple, low-cost ink-jet printers with more and more demand for high quality. Today, over 100M ink jet chips are produced every year and it is one of the major commercially-viable MEMS "success stories". [1-3] A detailed historical review on ink-jet technology can be found in [2-1]. The majority of activity in ink jet printing today is in the drop-on-demand methods. Most, if not all, of the drop-on-demand ink-jet printers on the market today are using either the thermal (TIJ [2-2]) or piezoelectric (PZE [1-1] pp. 570-578) principle [2-1].

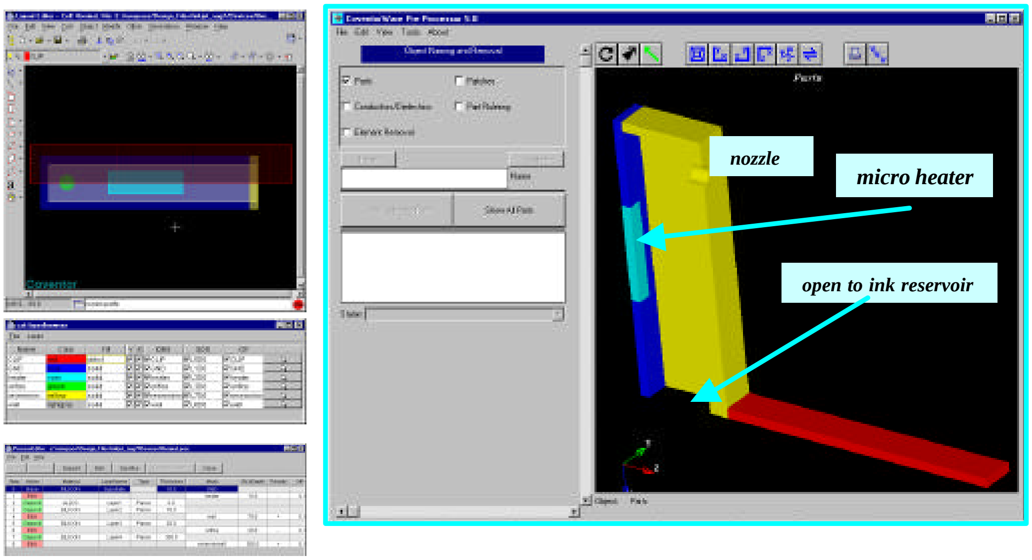


Fig. 2-1: Thermal ink-jet simulation: creating solid device model. Left Top: lay out masks. Left Bottom: design fabrication process. Right: geometry of the device.

Typical design questions are: (1) actuation profile (voltage verses time) coupled with geometrical dimensions: can a droplet be successfully ejected ? (2) quality of the droplets (volume, velocity and sphericity): will this droplet fly fast enough and remain spherical ? (3) droplet/paper impingement and dynamic spreading: will I get a good dot on the paper ?

DropSim™ based design analysis can be a guide to design solutions. Next, thermal bubble actuation and piezoelectric actuation are used as examples to illustrate the methodology.

The complex physics of nucleation and vapor bubble explosion makes it extremely difficult, if not impossible, to directly simulate the vapor bubble's life cycle. However,

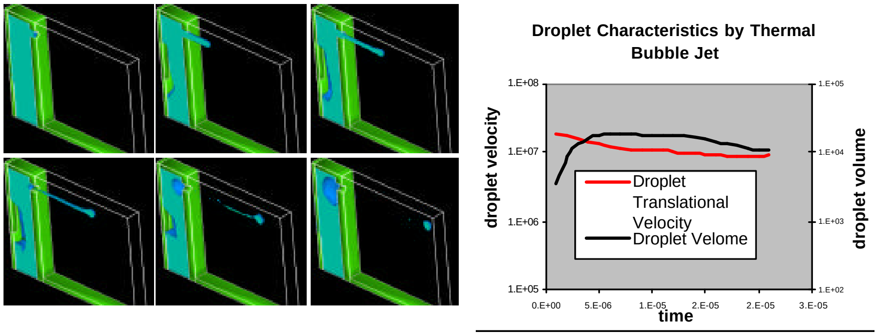
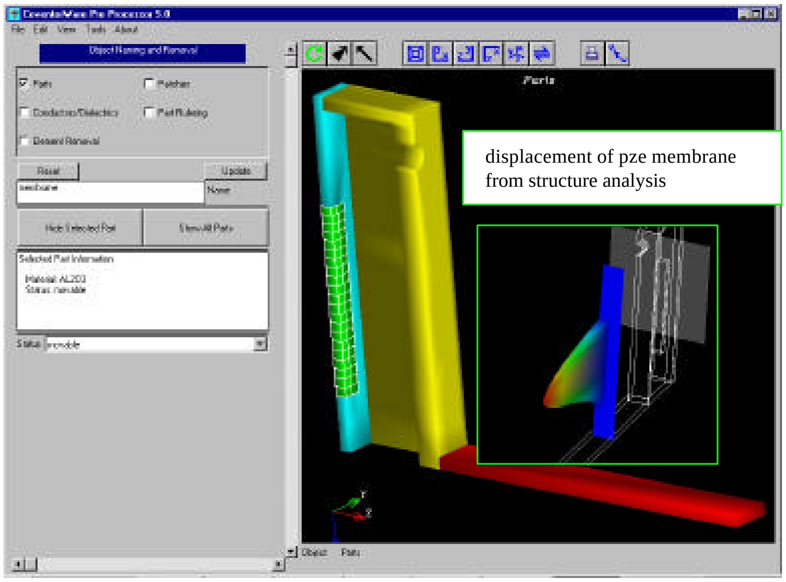


Fig. 2-2: Thermal ink-jet simulation: transient solutions of ink droplet ejection. Notice the life cycle of the vapor bubble close to the micro heater.



Selected Part Information

Material: AL2O3
Status: movable

Status: movable

displacement of pze membrane from structure analysis

Fig. 2-3: Device structure of piezoelectric ink-jet printing head. Displacement of PZE membrane is characterized by structure analysis and as input to droplet ejection simulation.

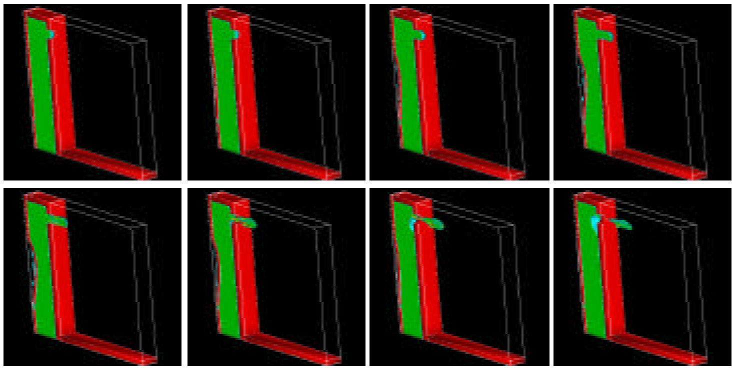


Fig. 2-4: Transient solution of droplet injection by membrane with prescribed motion.

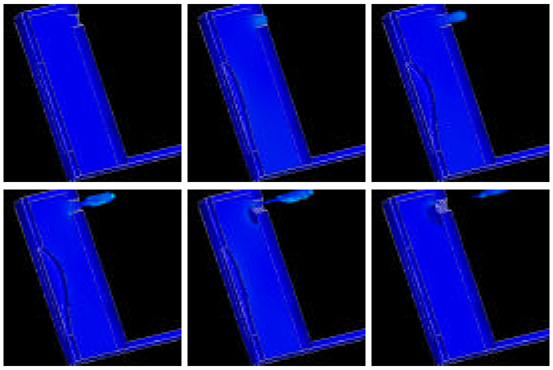


Fig. 2-5: Transient solution of droplet ejection by membrane with prescribed motion zooming at the moving membrane.

designers may extract the history of vapor bubble pressure from experiments and combine it with analytical analysis as ***DropSim*** ™ simulation input. Fig. 2-1 illustrates the simulation of the device fabrication: drawing masks, designing fabrication process and presenting the final device geometry. Fig. 2-2 presents the transient solutions of the ink droplet injection and the life cycle of the vapor bubble.

Direct simulation of piezoelectric driven inkjet printing requires fully coupled analysis across several domains of physics including piezoelectrics, structural analysis, fluid-structure interaction and multi-phase fluids. An alternative approach is to extract the PZE membrane behavior from experiments or a structural analysis simulation then using that as ***DropSim*** ™***/BubbleSim*** ™ input to drive the droplet ejection, as indicated by Fig. 2-3. Fig. 2-4 and Fig. 2-5 demonstrates typical simulation solution.

Reference

[2-1] Le, H. P., Journal of Imaging Science and Technology, Vol. 42, No. 1, 1998, pp.49-61

[2-2] Asai, A., Journal of Heat Transfer, Vol. 113, Nov. 1991, pp. 973-979

[2-3] Asai, A., Journal of Fluids engineering, Vol. 114, Dec. 1992, pp. 639-641

3. Design Applications II: Lab-on-a-Chip

One of the major MEMS application areas is micro-fluidic devices, or bio-MEMS, mainly used by pharmaceutical researchers. Micro-fluidic devices enable researchers to conduct biochemical reactions on a chip (micron-scale integrated chemical/biochemical analysis or synthesis systems, also referred to as Lab-On-a-Chip) that are traditionally executed in a laboratory. This technology has fundamental impact on both research and medicine. It increases the efficiency of experimental analyses whether in mapping a genome or in diagnosing and treating diseases. [3-1]

As Lab-on-Chip addresses more complex analysis problems, it requires more sophisticated micro-fluidic designs and control strategies. Elucidating the mechanisms that govern biological fluid flow is far from trivial. In this low Reynolds number regime, effects that are traditionally ignored gain importance due to the enormous surface to volume ratios in the device and due to the similarity in scale between the macro-molecule and the MEMS channel; surface tension becomes a major factor.

To achieve such elaborate goals, CFD based design and analysis for prototyping and refining micro-fluidic layouts become indispensable: it provides significant insight into the fluid mechanics in these systems in a quantitative way which enables the extraction of key parameters from improved or optimal operation of common micro-fluidic components.

Sample applications shown below illustrate the functionality and methodology of CFD analysis.

Reference

[3-1] Fortune, Oct 11 1999, pp.282[C]-pp.282[T]

3.1 capillary gating valves

Sample injection and localization are two essential functions required in such devices as samples must be first injected into the system and properly routed to a specific reaction chamber [3-1-1] [3-1-2]. These two functions can be accomplished for example using a series of valves that control the extent and flow of the sample. Other applications where micro-valves can be used to enhance on-chip chemical processing include improving the storage of reagents, priming of channels, switching of liquid flow-streams as well as isolating specific areas of the chip during sensitive steps in the chemical processing to prevent leakage and pressure fluctuations. From the device-design point of view, such valves are required to be easily connected to the fluidic networks, and also be able to bear high liquid pressure.

A passive micro-fluidic capillary-driven valve that exploits the surface tension force to stop flows in micro-channels recently has attracted considerable attention [3-1-4,5,6,7] and has strong appeal for

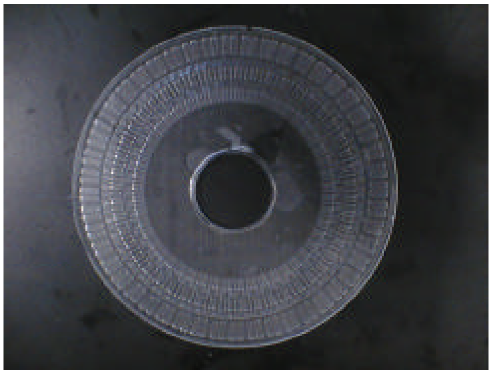


Figure 3-1-1: A micro-fluidic device where capillary-driven valves are used for fluid sample control. This device is fabricated by Tecon Boston (formerly Gamera Bioscience). Courtesy Dr. Gregory J. Kellogg.

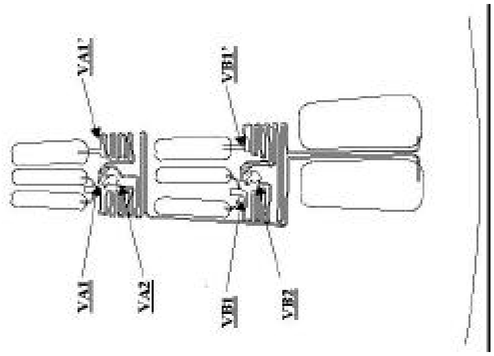


Figure 3-1-2: A slice of detailed micro-fluidic structure of the Gamera CD device positioned on the rotating plate radically. Fluids flow and combine from the reservoirs at top in two stages, gated by the junctions marked with the "V"s. (courtesy Dr. Gregory J. Kellogg).

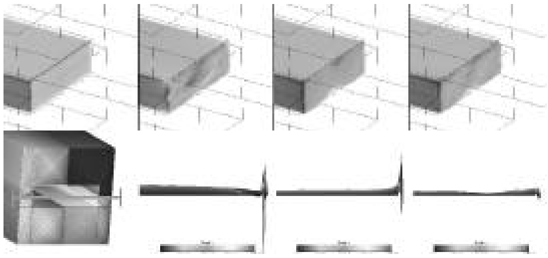


Figure 3-1-3: A typical transient process of meniscus formation (simulation results). Top row shows the shape of the meniscus, bottom row shows pressure distribution at a slide plane.

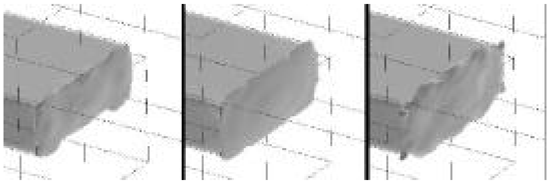


Figure 3-1-4: Breaking the capillary barrier. The driving pressure ? ? $^{?}$r ? r = 1719.12 Pa. From left to right the non-dimensional time is 1.17, 1.62 and 3.10.

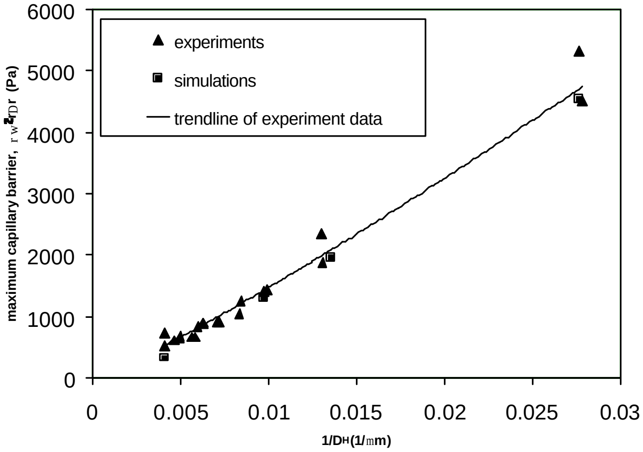


Figure 3-1-5: Maximum Capillary barrier verses geometry of the opening (comparison between simulations and experiments).

applications to various micro-fluidic systems. These valves have the advantage of not requiring moving parts. They are not sensitive to the properties of the buffer/samples pumped or the presence of trapped air bubbles. They also alleviate problems associated with Joule heating that occur in electro-kinetic systems that demand high field strengths.

The principle of operation is based on the pressure barrier that develops when the cross section of the capillary expands abruptly. As the meniscus (interface) area/volume enlarges with increasing driving pressure, the increase in interfacial surface energy appears as an equivalent capacitance in the fluidic circuit. This fluidic capacitance relates meniscus area to driving pressure in a similar way as electrical capacitance relates charge to voltage. Such a capacitance model requires the relation between the charge (driving pressure) and response (area of the meniscus). When the driving pressure exceeds a specific breaking point - the maximum capillary barrier - a fluid flow will be established through this micro-fluidic valve shorting the fluidic capacitance. The maximum capillary barrier defines the ceiling criterion of the capacitance working relation, another essential component of the fluidic capacitance model.

An example highlighting the capillary barrier extraction using ***DROPSIM^{TM}/BUBBLESIM^{TM}*** is a capillary-driven valve pumped by centrifugal force. Centrifugal driven Micro Total Analysis devices (for instance, Fig. 3-1-1) have attracted attention recently and become one of the major themes in contemporary lab-on-a-chip research [3-1-1]. A typical device consists of several structures such as in Fig. 3-1-2. distributed radially on a rotating disk [3-1-6]. The device is composed of fluid reservoirs, transport channels and reaction chambers. When the plate rotates, the centrifugal force builds up a pressure gradient inside the liquid with maximum liquid pressure at the meniscus.

The transient meniscus formation process is shown in Fig. 3-1-3. The top row shows the meniscus shape at the opening. A slice plane is cut through the liquid body from the meniscus to the reservoir. The bottom row shows the pressure distribution at that slice plane. To identify the maximum capillary bearing, the rotation speed is gradually increased until the liquid sample breaks the capillary barrier and floods into the reaction chamber, as shown in Fig. 3-1-4.

The maximum capillary barrier strongly depends on the dimensions of the capillary opening, represented by D_H, the hydraulic diameter of the opening. The dependency of the yield maximum capillary barrier on D_H is shown in Fig. 3-1-5. The simulation results are plotted against experimental data [3-1-6]. The experiments and simulations agree quite well as the figure shows.

Since the hydraulic diameter is chosen as the characteristic length, one would expect that the geometry of the opening would not have a significant effect on the capillary bearing pressure. Simulations were conducted to verify this dependence. (Fig. 3-1-6)

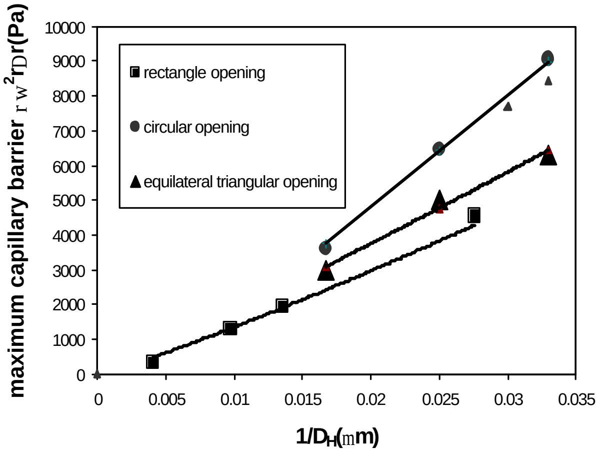


Figure 3-1-6: Maximum capillary barrier verses devices with capillary opening of different geometrical shape (simulation results).

Reference

[3-1-1] Van den Berg, A., Olthuis, W. and Bergveld, P., 2000, Eds. "Micro Total Analysis Systems 2000", Kluwer Academic Publishers

[3-1-2] Harrison, D. J. and van den Berg, A., 1998, Eds. ""Micro Total Analysis Systems '98", Kluwer Academic Publishers

[3-1-4] Man, P. F., et al, 11th Annual International Workshop on Micro Electro Mechanical Systems, Heidelberg, Germany, January 25-29, 1998

[3-1-5] Moroney, R., M., et al, 2nd International Conference on Modeling and Simulation of Microsystems, San Juan, Puerto Rico, April 19-21,1999

[3-1-6] Duffy, D. C., et al, 1999, Analytical Chemistry 71, 20

[3-1-7] Zeng, J., et al, Micro Total Analysis Systems 2000, Kluwer Academic Publishers, pp. 579-582

3.2 capillary filling

Lab-on-Chip usually consists of channels with complex shapes and cross-sections. Due to different fabrication techniques (for instance, isotropic wet chemical etching), the cross-section of the channel can be semi-circular, taped with certain angle (for instance, 54.7 degree [1-1] p.63) or of Gaussian curve. In order to achieve maximum length within a fixed "footprint" or other chemical sample transportation/mixing/reaction constraint, the channel path is usually curved with complex shapes such as a serpentine. A consequence of such a uniqueness of channel design is the so-called capillary filling problem: what geometry and under what kind of operation condition the chemical sample liquid can be injected into the channels *without* entrapping a gas bubble.

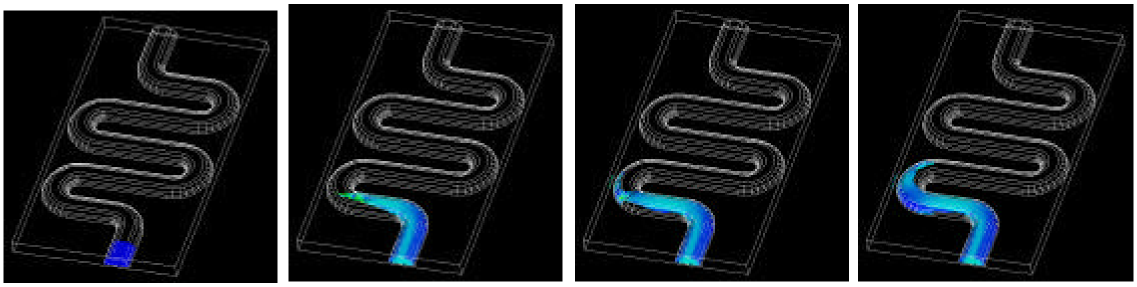


Fig. 3-2-1: ***DROPSIM***^{TM}***/BUBBLESIM***^{TM} simulation shows that gas bubbles are entrapped when the filling pressure is high. Shown above is a transient sequence of filling process of liquid chemical colored by velocity magnitude.

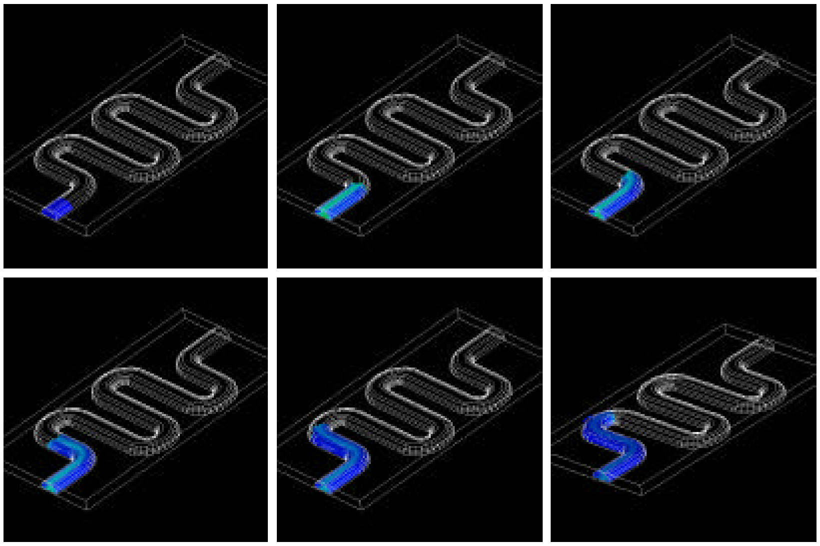


Fig. 3-2-2: When the filling pressure is lower, the interface advances gradually. Flow3d simulation shows there is no air bubble entrapped.

CFD simulation can assist design engineers to tackle this problem, as illustrated below. It should be noted that the liquid flow is dominated by surface tension force. It is critical that the simulation tool resolve the dynamic contact line problem accurately [3-2-1].

Reference

[3-2-1] Hirt, C. W., 3rd European Coating Symposium (ECS '99), Sept. 7-10, 1999

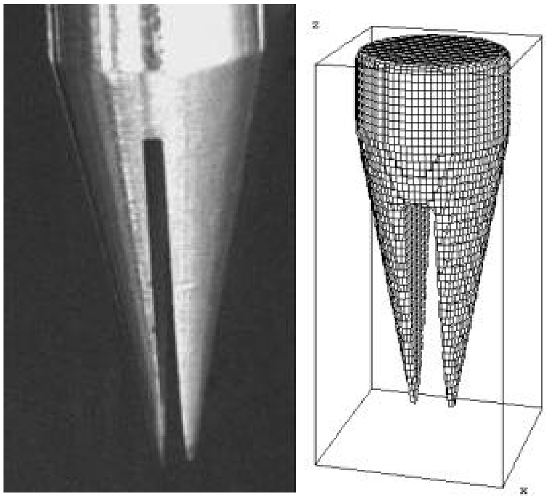


Fig. 3-3-1:At left is a split-pin fabricated by Brown group. A fine slot is machined into the end of the pin to accommodate liquid sample (courtesy professor Patrick O. Brown, Stanford University). At right shows solid structure and meshes used in numerical simulations.

4. Design Applications III: Micro Arraying

Microarray technology was first introduced by the Brown and Davis groups [3-3-1][3-3-2][3-3-3] to deposit pre-synthesized oligonucleotides or PCR products onto solid substrates. The substrates are then processed and analyzed in parallel. This powerful technology enables the simultaneous analysis of thousands of sequences of DNA, and has found wide use in genomics (for instance, [3-3-4]), and more recently, in proteomics [3-3-3].

Pin based liquid sample deposition (spotting) is widely employed due to its low cost, simplicity and robustness[3-3-1]. Figure 3-3-1 shows a split-pin fabricated by the Brown group. The pin is first dipped into the sample solution and a small volume of fluid is transferred into the slot. The pin is then guided to "tap" the substrate leaving a spot of the sample. The tapping force required to deposit a sample spot on the substrate is not insignificant [3-3-1]. Such direct contact can lead to mechanical damage to the pin tips. In addition, the sample droplet volume is affected by the speed at which the pin strikes the surface (for example,2cm/sec [3-3-1]), which depends on the local mechanical contact property of the substrate - it can therefore be a major source of droplet volume disparity.

A split-pin based non-contact spotting method is described here, that uses precise control of the pin trajectory. The displacement of the pin in the spotting sequence is shown in Figure 3-3-2 using ***DROPSIM***^{TM}/***BUBBLESIM***^{TM}. The sample spot is deposited on the surface without tapping, by triggering the required instability to break the droplet through the acceleration of the pin away from the substrate. This approach overcomes the disadvantages of the conventional approach described above. This spotting approach enhances the uniformity of the volume of sample spots. Furthermore, it offers a new mechanism to actively control the spot volume, or *spotting-volume-on-demand*. This can be accomplished by adjusting the pin's pulling velocity – spot sizes from 1-1000 pL can be deposited as shown in Figure 3-3-3.

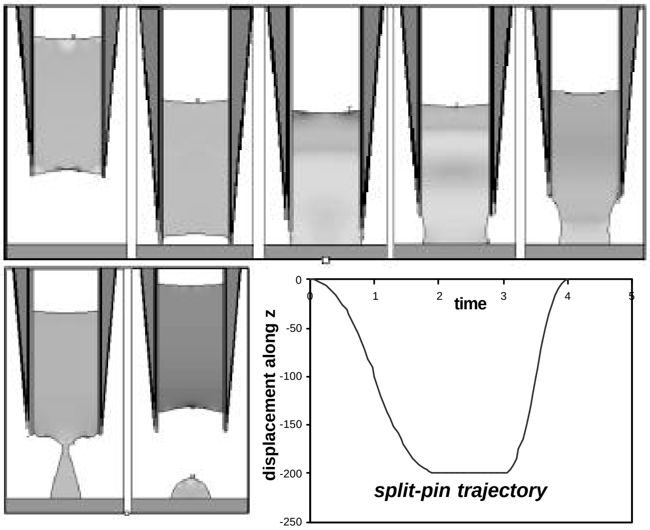


Fig. 3-3-2: Time sequence of liquid sample spotting. Motion of the split-pin is defined as shown trajectory. Frames are corresponding to 0, 1.8, 3.3, 3.5, 3.6, 3.8, 4.0 milliseconds. Minimum distance between pin tip and substrate is 2 μm.

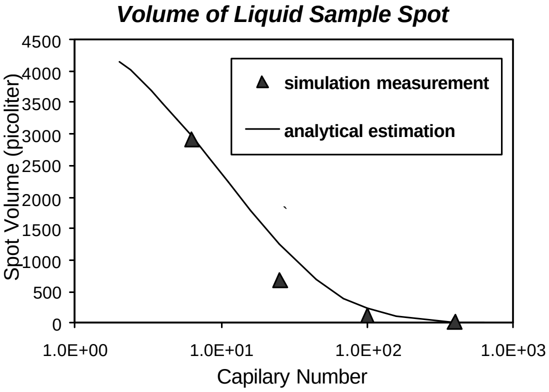


Fig. 3-3-3: Adjusting pin's pulling velocity can actively control the spotted liquid volume. Measured results are from numerical simulation, which agree with analytical estimation.

Reference

[3-3-1] Rose, D., in "Microarray Biochip Technology", edited by Mark Schena, Eaton Publishing, 2000

[3-3-2] DeRisi, J. L., Iyer, V. R. and Brown, P. O., Science 278, pp.680-686, 1997

[3-3-3] Tseng, F. G., et al, ASME MEMS 2000, Vol. 2, pp.659-663

[3-3-4] Genetic MicroSystems, GMS 417 Arrayer User Guide, 1999

[3-3-5] Zeng, J., et al, Micro Total Analysis Systems 2001, Kluwer Academic Publishers

5. Design Applications VI: Micro-Opto-Electro-Mechanical Systems

Explosive data growth is changing the landscape of the network: it has never been so hungry for bandwidth. This demand is encouraging a new breed of technologies to make networks faster, more reliable, and more scalable than ever before. One of these technologies is the optical switch.

Blowing a microscopic bubble into a switch using a micro heater causes the light to make a right turn. The absence of a bubble in the junction of the switch let the light beam proceed straight. [4-1] This Agilent Bubble Switch is one of the most publicized optical switch technologies utilizing microfluidics. Furthermore, microfluidic optics application is not limited to micro bubbles : Agilent Bubble Switch reveals that the interface between vapor and index-matched liquid can cause the light to bend and move into another waveguide *just like a micro mirror*.

It is of importance to understand the behavior of the interface with respect to the mechanism that actuates the interface. A design question is how strong the actuation should be so that the interface moves fast enough to achieve the specified optical switch frequency. CFD simulation can help to guide designers in search of a solution.

Fig. 4-1 illustrates a mechanism of operation of an example microfluidic switch. It utilizes the Marangoni effect to create the switch. Fig. 4-2 shows a ***DROPSIM***^{TM}***/BUBBLESIM***^{TM} simulation of a liquid plug swimming to the cold end along a channel creating a desired vapor regime at the cross-section of the waveguide.

Reference

[5-1] Bishop, D. J., Scientific American, January 2001, pp. 88-94

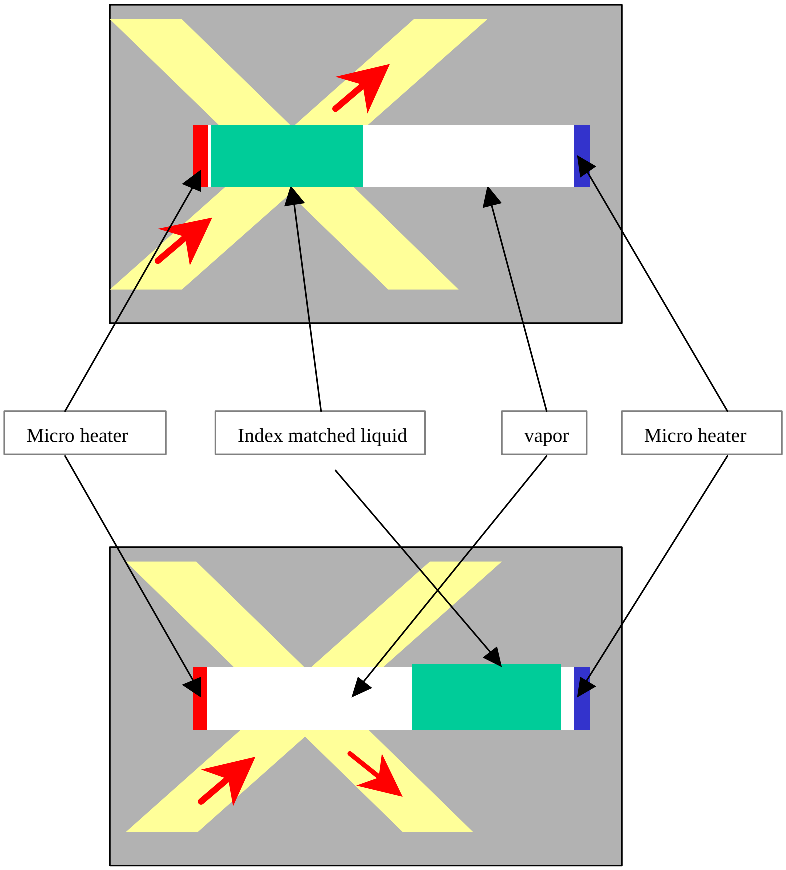


Fig. 4-1:A plug of liquid is placed at cross-section of light path. Since the liquid is index matched, the light passes through (cartoon at top). Two micro heaters are mounted on the two-end of the channel creating a temperature gradient along the channel length. The surface tension coefficient decays when temperature goes higher therefore the liquid plug swims to the cold end (micro heater B) leaving vapor at the light path cross-section which bends the light entering another fiber.

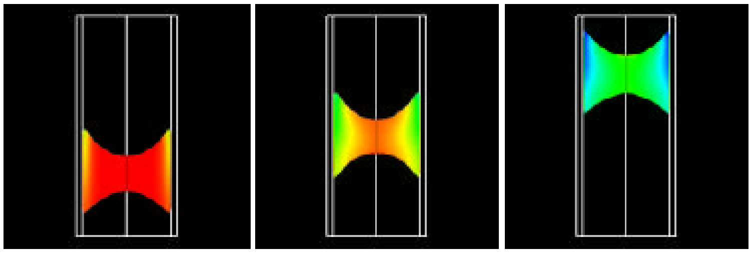


Fig. 4-2: an index-matched liquid plug swims to the cold end, a sequence is shown, liquid is colored by temperature (***DROPSIM***^{TM}***/BUBBLESIM***^{TM} simulation).