

NUMERICAL AND EXPERIMENTAL ANALYSIS OF MICROFLUIDIC DEVICES MANUFACTURED IN LTCC

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Abstract. *The mixture of fluids and reagents constitutes basic stage in many processes in industry and applied science, with applications in Medicine, Pharmacy and Analytical Chemistry. Microfluidic systems and devices display advantages as portability, small volumes of samples and continuous production. Microfluidic mixers with channel size from 1 mm to 1 μ m, and flow speed typically of 1 m/s are being used for several applications. Reynolds number is smaller than 1000, characterizing laminar flow regime. Thus, in micro scale the mixture of fluids is dominated by diffusion mechanism, which is a slow and inefficient process. It is possible to speed up this process, by means of active and passive microfluidic devices.*

In this work an active and passive microfluidic mixers are considered. Devices are implemented in LTCC (Low Temperature Co-fired Ceramics) technology, driven by ultrasound where the mixing is done by mass transport. Passive devices are implemented using micro-channels with sharp bends and steps generating a 3D geometry. Analysis of micromixers with channels implemented in LTCC using finite element models were performed using different fluids with distinct densities and piezoelectric ceramic actuators working in different resonance frequencies and voltage excitation magnitudes. Experimental results for pressure loss and speed gain are also presented.

Keywords: *Micromixer, Mixing, Microfluidics, Finite Element analysis, Ultrasound.*

1. Introduction

In the last decade Microfluidics has been accepted as an emergent and interdisciplinary technology serving as a tool in diverse applied science areas. Nam-Trung (2002) shows that in the late 80's, the scientific production related to microfluidics was of approximately 20 papers published in international journals and conferences; in early 2000 this number grew to about 150 articles published. The sales of microfluidics devices and systems has also jumped from US\$500 million in late 90's for ~US\$3.5 billion dollar in 2003.

Microfluidics is a branch of Microtechnology that involves the research and development of micro-scale devices that can handle small volumes of fluids, with focus on controlling the flow of liquids and gases in systems with dimensions of the order of microscale. For external flow control there are speed and turbulence control sensors, for internal flow control there are microvalves, micropumps and microsensors.

The advantages of microfluidics devices are: portability, integration of process and instrumentation, small sample amounts, low processing time, continuous process, better control and reliability, lower energy consumption and reduction of manufacturing costs in mass production. Applications range from process intensification to life sciences, with devices for diverse applications such as: microneedles, microdispensers, microfilters, microseparators, microreactors and micromixers.

In particular, micromixers present a wide range of applications in industry and research. A fast and efficient mixture becomes necessary in situations such as drugs dosage, nucleic acids sequencing or synthesis, DNA sequencing, cellular activation and reactions with enzymes and proteins. In food and cosmetic industry mixing is a critical process phase.

Microfabrication technologies have played a crucial role in the development of microfluidics from its inception; flow characterization techniques and numerical analysis plays an important role. In the present paper we will present numerical studies and experimental measurements in micromixers manufactured using LTCC (Low Temperature Co-fired Ceramics) technology, as described by Gongora-Rubio et al (2001).

2. Mixers

The mixture of fluids and reagents constitutes a basic step in industry and science. Macroscopically, mixing is carried out in turbulent and convective flows in batch operations. In this kind of flow individual movement of fluid particles overlaps average movement, causing a bigger interaction of fluid layers, thus, improving mixing. This kind of operation has the disadvantage of working with great volumes, resulting in larger processing time for mixture homogenization; furthermore, there are material losses as wall deposits in macromixers.

Microscopically, mixture happens in laminar flows, where the dominant process in mixing is molecular diffusion. The average movement of fluid layers governs the flow. They flow in parallel, without mass transport in the radial flow direction, except for small molecular diffusion, between layers, thus, becoming an inefficient process.

However, it is possible to improve drastically mixing efficiency in microscale improving the device engineering. There are two groups of micromixing devices found in the literature: passive and active micromixers. In passive micromixers mixture is carried out due to flow disturbances generated by device geometry. Active devices actuation is through an external power source that introduces flow disturbances in order to improve mixing.

2.1. Passive Micromixers

Let's consider a micromixer formed of two entrances and a straight channel with cross section of 1 x 1 mm, with hydraulic diameter (D_h) of 1 mm, pure water at 20 °C flowing at 1 m/s, with water specific mass of $\rho = 998.2 \text{ kg / m}^3$ and dynamic viscosity of $\eta = 1.002 \times 10^{-3} \text{ Pa}\cdot\text{s}$, Reynolds number can be calculated as:

$$Re = \frac{\mathbf{r} \cdot \mathbf{v} \cdot D_h}{h} = \frac{998.2 \cdot 1 \cdot 1 \cdot 10^{-3}}{1.002 \cdot 10^{-3}} = 996.2076 \quad (1)$$

The Reynolds number obtained indicates a laminar flow regime, characterized by organized and parallel movement of fluid layers; there is no flow between fluid layers. Due to this characteristic, mixture process in a straight channel is dominated by molecular diffusion, so we have an inefficient and unproductive mixing process.

However it is possible to improve mixing process disturbing the fluid layer flow in microchannels and increasing diffusion between species, generating the following effects: increase of contact surface between fluids, creation of bi or three-dimensional velocity fields, generation of recombination regions, generation of transversal flows or generation of chaotic movement.

These effects are classified as: lamination, where the main flow is divided in n secondary flows and recombined m times; injection, where two or more fluids are injected in the device in order to obtain deep interaction and chaotic advection, with the basic idea of modifying the channel shape for splitting, stretching, folding and breaking of the flow. Devices with twisted 2D and 3D conduits present great potential for fluid mixing in microscale. Recently Liu R. H. et al (2000) showed an experimental comparison between three devices: straight channel, square wave channel and 3D serpentine channel. The devices present channels with cross section of 300 x 150 μm . Using different fluids, Liu, showed that serpentine 3D micromixer produced 16 times more reaction than the straight channel and 1.6 times more than the square wave micromixer.

Liu Y. Z. et al (2004) compares three devices using computational simulations: square wave channel, serpentine 3D channel and channel with cavity. The dimensions of the cross sections are 300 x 150 μm for the square wave channel and 3D serpentine channel and 360 x 139 μm for the channel with cavity. The 3D Serpentine micromixer was shown to be more efficient than the other two devices for Reynolds number ranging from 1 to 100.

Gongora-Rubio et al (2005) shows the potential of 3D serpentine micromixers in the preparation of polymeric microspheres. The fluids used were a solution of polyvinyl alcohol (PVA) in water and a solution of Eudragit RS100 in ethyl acetate (EA). Devices with cross sections with hydraulic diameter of 897 μm and 575 μm were used. It was found

that when channel hydraulic diameter is reduced, drop dispersion is quite reduced. Further drop dispersion reduction was obtained increasing effective channel length and flow rate.

The present work examines micromixer structures with twisted 2D and 3D conduits in different configurations, and compares them with a straight channel micromixer. Comparison parameters are: pressure loss, device size and flow velocity.

Pressure loss is an important parameter for feeding pump sizing; therefore structures with low pressure loss were preferred. Flow velocity speed is important in 2D and 3D structures because flow disturbance and fluid layers interaction is increased.

Six micromixers were manufactured in LTCC: one with a straight channel and five with different 2D and 3D configurations, all with cross sections of $600 \times 600 \mu\text{m}$, chosen arbitrarily. For comparison all the structures have the same effective channel length of 48 mm.

In this work devices are identified as: straight channel micromixer (DM1), zigzag 2D micromixer (DM2), square wave 2D-XY micromixer (DM3), square wave 3D-XZ micromixer (DM4), zigzag 3D micromixer (DM5) and serpentine 3D micromixer (DM6). Figure 1 shows fabricated devices layout.

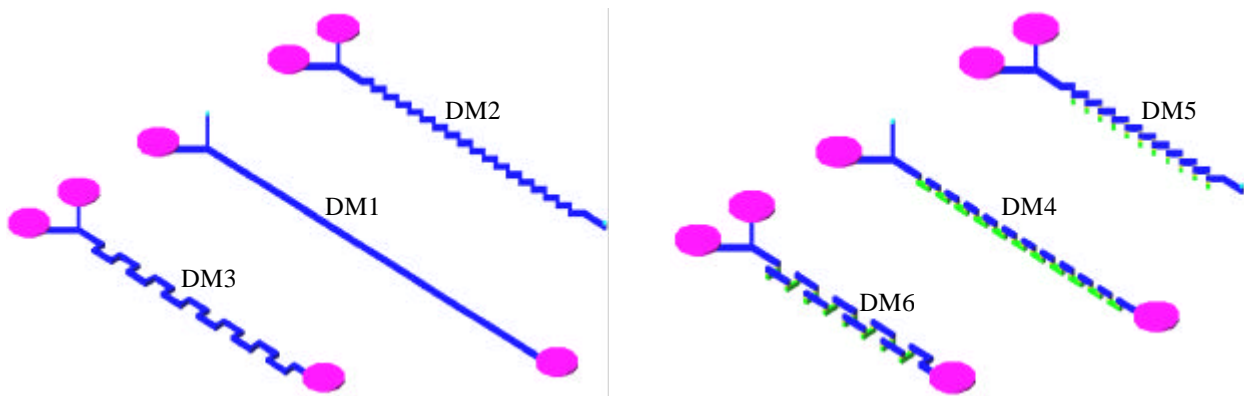


Figure 1. Proposed passive micromixers.

2.2. Active Micromixers

In active micromixers, an external energy source generates flow disturbances for improving mixing. There are several physical principles for generating such flow disturbances: pressure gradients, electrohydrodynamics, electrophoresis, electrokinetics, magnetohydrodynamics, acoustics and thermal, as shown by Nguyen and Wu (2005).

Yang Z. et al (2001) introduced an ultrasonic micromixer manufactured in silicon, with piezoelectric (PZT) ceramics exciting a diaphragm below a silicon chamber, using a square wave signal with 50 V peak-to-peak and 60 kHz frequency.

In the present work also we will model channel cross sections to study the effect of ultrasonic vibrations in fluids, with interest in the following parameters: frequency and peak the peak ceramic excitation voltage.

3. Fabrication Techniques

Low-temperature co-fired ceramic (LTCC) tape technology was developed for efficient manufacturing of monolithic packages and hybrid microelectronics circuitry. Note that the size of our intended device is in the meso-scale range, between tens of micrometers to few millimeters. This size range is ideal because there is no need for a clean room and instrumentation is inexpensive as compared to pure semiconductor fabrication.

The Green tapes are glass-ceramic composite materials. The usual composition also includes a glass frit binder to lower processing temperature as well as rendering the material compatible with thick film technology, and an organic vehicle for binding and viscosity control. They are commercially produced in flat tapes of various thicknesses but usually in the range of 100 to 300 μm . They are called green ceramic tapes because they are manipulated in the green stage; that is before firing and sintering.

One of the important features of green tape technology is the possibility of fabricating three-dimensional structures using multiple layers of green tapes.

The processing of the green ceramic tapes is usually done in three basic steps:

- Patterning of individual layers with via holes, resistors, conductors, dielectric pastes, depending on application;
- Collation and lamination of the tapes under pressure and temperature;
- Co-firing of the entire laminate to sinter the material.

The typical processing schedule for LTCC microfluidic devices is shown in Figure 2.

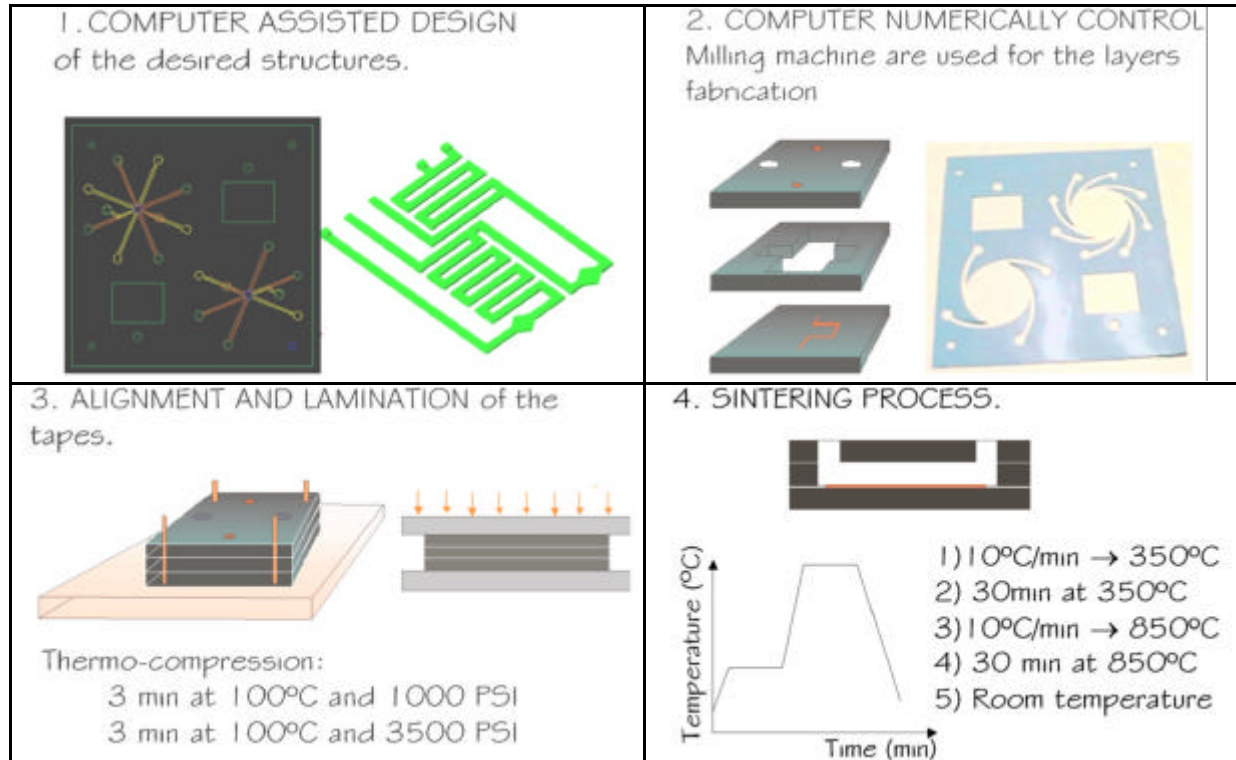


Figure 2. LTCC processing steps for a microfluidic device.

4. Computational Models

The computational models were based on the ANSYS finite element software. CFD FLOTTRAN module with FLUID142 3-D Fluid-Thermal element was used to model 3D devices. It is a tetrahedral element that presents the following degrees of freedom: speed in x, y and z directions, pressure, temperature, turbulent kinetic energy and turbulence dissipation rate.

The devices models totaled between 60000 and 80000 hexahedral elements with sides approximately 75 μm long. The boundary conditions adopted are: zero velocity at walls, zero exit pressure and flow velocity at inputs; the work fluid was pure water. The analysis was carried out for four different velocities in laminar flow regime obtaining results of pressure loss and flow velocity fields.

For ultrasonic vibration influence on the flow, ANSYS was used as well, using three elements: PLANE13 from coupled field module, PLANE42 from structural solid module, and, FLUID29 from fluid module. 2D analysis was performed for steady and transient states.

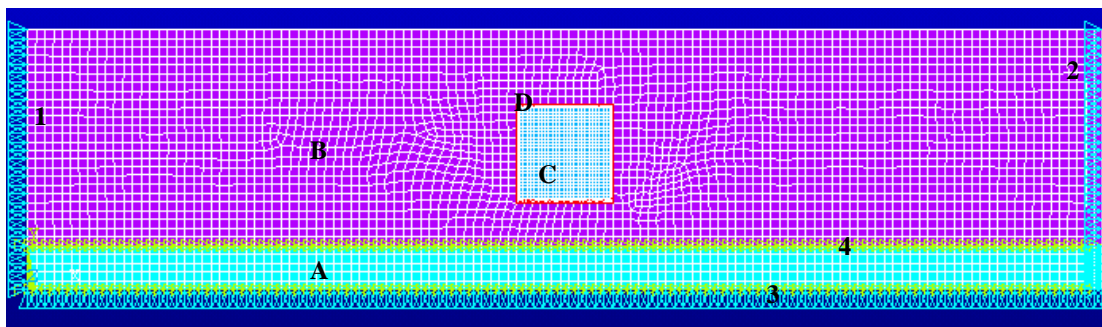


Figure 3. Model used for ultrasonic vibrations effects in fluids studies.

In Figure 3 a model used for ultrasonic vibrations influence on flow analysis is shown: area A is piezoelectric ceramic with PLANE13 element used, area B is (LTCC) green ceramics substrate, with PLANE42 element used, area C

is the fluid channel with FLUID29 element and area D uses FLUID29 element but allowing for fluid-structure interaction. In lines 1 and 2 displacement is restricted to x direction, in line 3 displacement is restricted to y direction. Piezoelectric ceramic excitation voltage, area A, is applied between line 4 and grounded by line 3.

5. Experimental Procedures

Pressure loss was measured by means of a differential capacitive pressure sensor (C719, Analcont) with micromixer input and output connected to the transducer inputs. Flow rate was imposed using a syringe pump (74900-20 Syringe Pump, Cole Parmer). Several experiments were conducted in order to verify the structure with lowest pressure loss and flow velocity.

6. Results and Discussion

Figure 4 depicts flow details obtained for the devices analyzed and that the geometry may be used to increase flow disturbances. The introduction of elbows clearly creates regions with high velocities and vorticity, as shown in Figure 4a when compared to Figures 4b-4f. It can be noticed that structure DM2 (Figure 4b) is better than other structures (Figure 4a and Figures 4c-4f), which is confirmed by numerical results on Figures 5a and 5b.

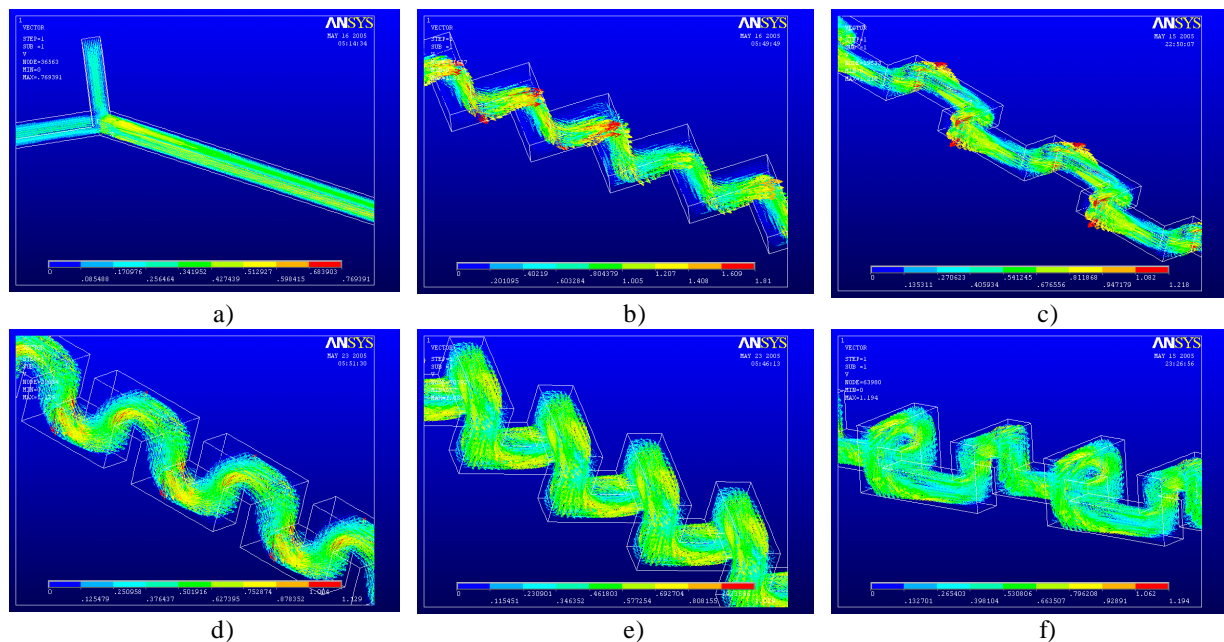


Figure 4. Flow details in studied devices: a) DM1, b) DM2, c) DM3, d) DM4, e) DM5 e f) DM6.

It is observed in Figure 5a that structure DM2, with successive elbows, presents a higher velocity than that observed in the straight channel structure (DM1). A better performance is expected for the DM2 structure since in disturbed flows mixing is related to maximum vorticity (and therefore maximum velocity since the velocity at walls is zero). On the other hand, the pressure loss of DM2 is higher than the loss of DM1 as shown in Figure 5b resulting on the need of a feeding pump with larger capacity for structure DM2. To improve mixing on DM1, the flow rate should be decreased, which is not desirable since the flow rate is usually a project requirement.

The other structures analyzed present higher manufacturing complexity but they might represent a good option since they display velocities higher than DM1 but pressure drop lower than DM2.

Experimental results obtained for pressure loss with different flow rates and devices are shown in Figures 5c and 5d. The pressure losses of 3D devices (DM4 – DM6) were larger than those of 2D devices (DM1 – DM3). Experimental and numerical results of the straight channel DM1 agree well (see Figure 5c and 5d). However, experimental results obtained for 2D structures with elbows (DM2 and DM3) show a pressure loss less than numerical results. And the experimental results obtained for 3D structures (DM4 – DM6) shown a pressure loss larger than the numerical results. This effect might be explained by differences in surface roughness and geometry tolerances in these devices, which is not considered in the numerical model (well defined dimensions and smooth walls). These effects will be analyzed and characterized in future work.

A trade-off between mixing efficiency, low pressure loss and geometry complexity has to be explored, and depending on application different structures may be used.

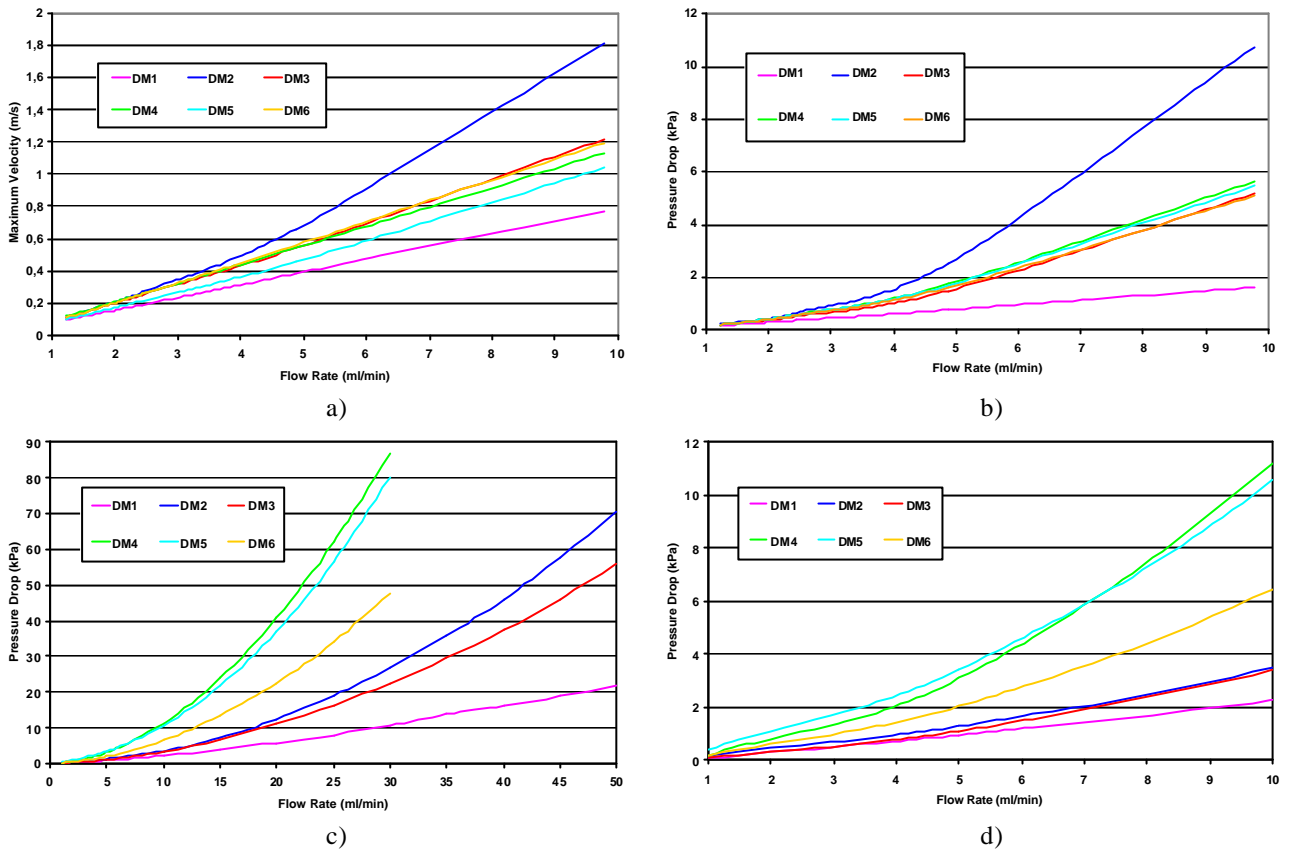


Figure 5. Numerical results for a) Maximum Velocity versus Flow Rate, b) Pressure Drop versus Flow Rate; and experimental results for c) Pressure Drop versus Flow Rate and d) Pressure Drop versus Flow Rate for 1 to 10 ml/min.

The use of active structures for mixing was also analyzed. The effect of ultrasonic vibrations in stagnant fluid inside channels with differing dimensions was studied. In Figure 6 is shown how the pressure at the center of the channel varies with ultrasonic frequency for different channel dimensions. The maximum pressure decreases for smaller channel dimensions. The frequency at which this maximum occurs initially increases for smaller channels but the two smallest channels do not follow this trend.

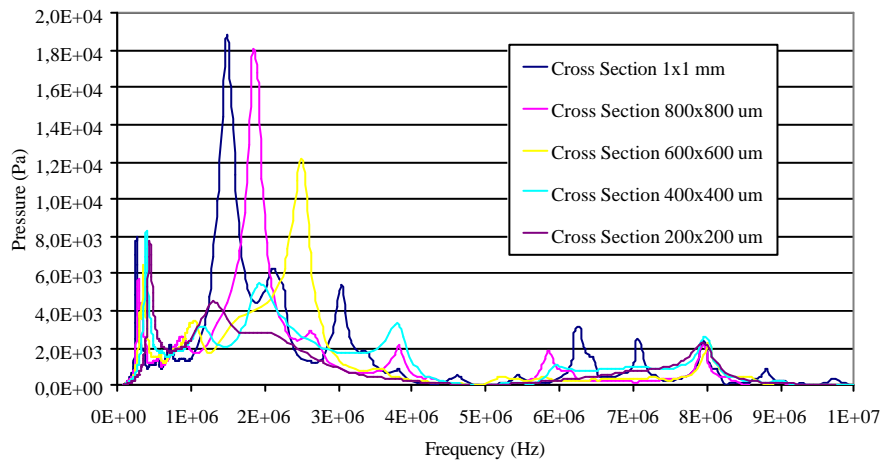


Figure 6. Numerical results for pressure magnitude versus frequency for several channel cross sections for a range of 1 Hz a 10 MHz.

For a channel with a section of 600 x 600 μm , pressure versus frequency for three different values of peak-to-peak excitation voltages are plotted in Figure 7a; a linear behavior of peak pressure for different voltages is observed. Results in Figure 7b show the pressure versus frequency for a transversal section of 600 x 600 μm now using two different

fluids, water and blood, and three different peak-to-peak excitation voltage, showing different behavior since the wave propagation speed is different in the second fluid.

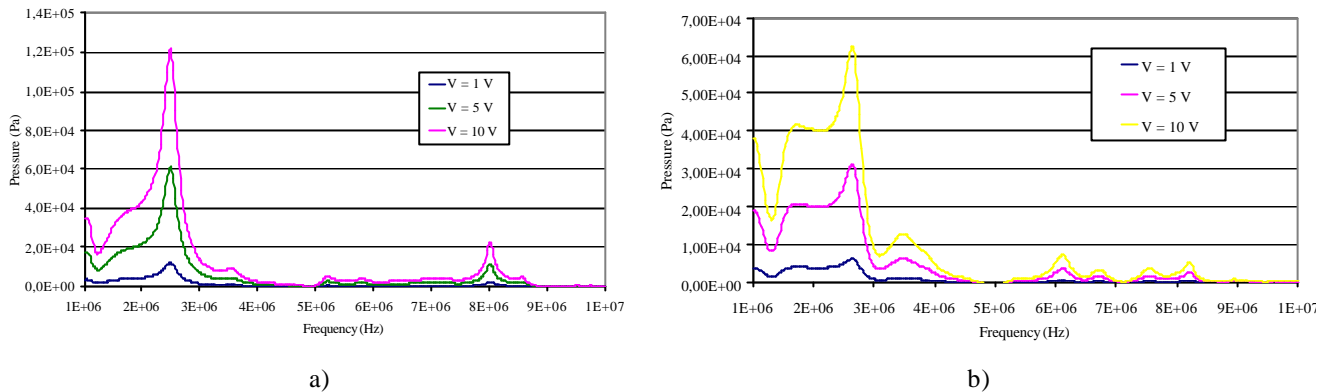


Figura 7. Numerical results obtained for pressure magnitude versus frequency for a cross section of 600 x 600: a) single fluid (water) and b) two fluids (water and blood).

In Figure 8 are shown the pressure contours for four different frequencies corresponding to the peaks found in the Figure 7a (for a given voltage). In Figure 8, pressure patterns (blue and red spots) can be noticed. The largest patterns are seen for the frequency corresponding to the peak pressure of Figure 7a. When the frequency is higher, the size of the patterns (blue and red spots) decrease in size. Smaller spots yield better mixing. On the other hand, large spots (such as Figure 8a) corresponds to a valve since the high or low pressure at single plane may decrease the flow rate.

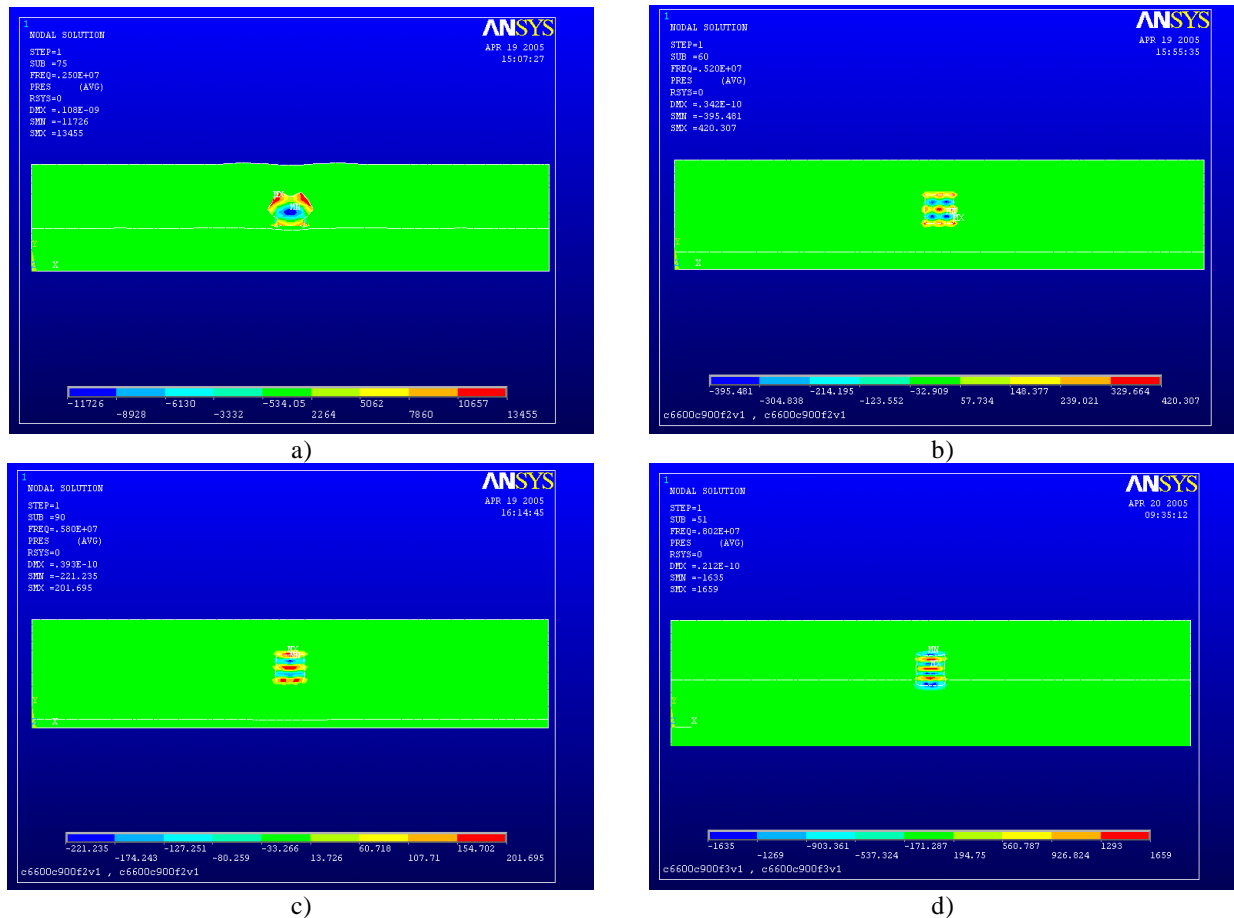


Figure 8. Pressure maps obtained by numerical model for single fluid at: a) 2.5 MHz, b) 5.2 MHz, c) 5.8 MHz d) 8.02 MHz.

7. Conclusions

Microfluidic devices with different geometries were studied to determine the effect of disturbances on the laminar flow to improve mixing of fluids. The effects of ultrasound excitement on the devices were also studied.

When comparing the numerical and experimental results, it is observed that results agree for the straight channel (DM1) since the flow is much simpler and fabrication tolerances are smaller; the pressure loss experimental results of two dimensional channels (DM2 and DM3) are lower than those obtained numerically. The three dimensional devices (DM4 – DM6) resulted in larger experimental pressure loss. This is probably due to wall roughness not modeled in the numerical simulations and difficulties in manufacturing the devices with small tolerances. Other problems in the numerical simulation should not be discarded. Three dimensional flows are very complex even when flow is laminar. Flow separation and other unsteady phenomena could exist that influences the numerical results.

Active flow disturbances using ultrasonic vibrations for mixing improvement was numerically studied. The parameters studied were frequency and peak-to-peak ceramic excitation voltage. The numerical results so far obtained show that ultrasonic excitation can be used, along passive techniques, to improve fluid mixing.

So far the actual mixing was not studied, only peak velocities and pressure distribution. The next step in this ongoing research is to study the actual mixing and discrepancies in experimental and numerical results observed.

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