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TECHNICAL BRIEF: NUMERICAL MODELING, ANALYSIS AND DESIGN OF VARIOUS MICROMIXERS

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Abstract- Manipulation, separation and detection of bio/chemical species in micro environment for laboratory purposes is demanding with an inexpensive lab on a chip device. Apart from time consuming laboratory analysis with high end technological instruments, computational analysis has been creating a breakthrough in custom design with a promise of better, efficient and low cost mass fabrication of micro fluidic devices. Low Reynolds's number flow in micro channel requires long diffusion length requirements which do not propose notable practical solutions. Here, we have used micro mixing by the use of electro osmotic effects applied through the walls of the microchannels. The use of different geometries, electrode positions and numbers, frequencies of ac potential and channel width has shown promise for effective mixing phenomena in micromixers. Circular micromixer model have shown a considerable decrease in concentration variance over time at the outlet which can be effectively optimized to have uniform mixing characteristics over time. As a continuation of our previous work to develop the effective micromixer, ionic fluid flow visualization tools including velocity contours, concentration contours, and velocity vectors are presented here.

Keywords- μTAS, Bio-MEMS, Mixing, Electro-osmosis, Geometric shape, Mathematical modeling, Numerical Solution, COMSOL Multiphysics.

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Introduction

Over several decades, microfluidics researchers have been looking to build a single lab-on-a-chip capable of performing multi-laboratory processes [1]. Mixing at micro-level is one of the fundamental laboratory processes required for varieties of biochemical applications including micro biochemical analysis, protein folding, polymer chain reaction, DNA hybridization, etc.

The mixing is primarily performed by diffusion at low Reynolds number and high Peclet number fluid flows. For these types of flow, uniform mixing requires to have long mixing length and longer mixing time to ensure satisfactory mixing phenomena. Several passive mixers have been reported in earlier studies [2,3]. Specific channel geometry in these micro mixers demonstrated better mixing performance of the species by increasing the interfacial contact area of the mixing species. Judicial interaction of magnetic and electric fields was also reported to enhance mixing phenomena [4]. The parametric studies of electroosmotic transport characteristics have also been studied [5]. Customized geometries of mixing channels are reported to enhance the mixing process [6]. Here we remodeled the shapes and varied the number of electrode pairs, mixing channel width and species concentration to investigate and optimize the mixing process using COMSOL, a commercial finite element software package [7].

Applying statistical measuring tool of variance for concentration mean values at the outlet, Concentration variances (S) vs. time at the outlet were compared for each of these models to determine their uniformity of mixing.

$$S = \int_0^y (c - \bar{c})^2 \, dy \qquad (1)$$

Where $\bar{c}$ is the concentration at any point at outlet and is the mean concentration.

Computational Modeling

The main control model i.e. a circular electro osmotic mixer encloses a toroid area within the 5μm and 15μm radii. The distance between the inlet and outlet extremities is set to be 80μm. Channel widths for inlet, outlet and mixing zones are all set to be 10μm taken from a published article and also as given in COMSOL model library [7,8]. All other shape modifications (i.e. square, and two elliptic mixers) were made as the continuation of our previous work provided that the same mixing width and same mixing area as shown in [Fig-1] [9]. An electrolytic species of 1 mol/m^3 concentration and a non-concentrated species (i.e. 0 mol/m3) separated at the midpoint along the longitudinal line of the inlet are injected into the channel with velocity (v) 0.1mm/s having the entrance length of 1 m. The two electrode pairs are positioned at angular positions of 45, 135, -45 and -135 degrees respectively with alternate polarity. These geometric micromixer models are then further preprocessed for meshing. Using COMSOL software package, free triangular meshing scheme with extra fine elemental size was used in all the mocromixer models. The proximities at electrode positions and incoming ports were custom meshed per maximum element size of 0.2 and 0.1 respectively with maximum element growth rate of 1.1 each.

At the walls of the channel, no slip boundary condition was applied. Slip boundary conditions were applied between the electrodes and the bulk solution. The fluid motion inside and outside the electric double layer is governed by (2) and (3,5) respectively. The slip velocity at the slipping wall is governed by (4). For the electrical input, sinusoidal voltage of 0.1V over time is applied across the electrodes with alternate polarity.

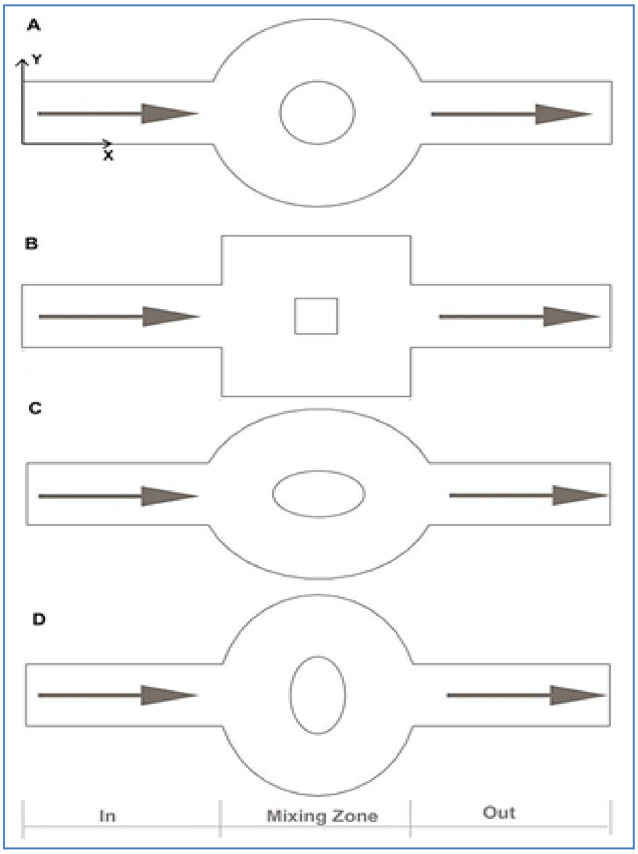

Fig. 1- Models of various electroosmotic mixers: (A) circular, (B) square, (C) elliptic-I and (D) elliptic-II mixers

Mathematical Modeling

The mathematical modeling is based on the following equations.

$$\rho\left[\frac{\partial u}{\partial t}+(u.\nabla)u\right]=-\nabla p+\mu\nabla^2 u+\rho_e \mathrm{E} \quad (2)$$

$$\nabla.u=0 \quad (3)$$

$$U_{slip}=-\frac{\varepsilon\zeta\mathbf{E}_x}{\mu} \quad (4)$$

$$\rho_e E=-\mu\nabla^2 \mathrm{V} \quad (5)$$

Where,

P_e: Charge density, **E:** Electric field intensity,

μ: Dynamic viscosity of fluid,

є: Permittivity of the medium,

ζ: Potential (0.1V) and

E_x: Electric field intensity.

Other physical parameters include the following: Conductivity of solution = 0.11845 S/m, Frequency of ac potential = 8 Hz,

Diffusion coefficient of the solution = 1×10^{-11} m2/s, Relative permittivity of fluid = 80.2

Results and Discussion

Surface Concentration Contours in the Microchannel and Concentration Variance at the Outlet

The applied electric fields perturbed the streamlines of velocity field over time and concentration variance vs. time were earlier reported in our previous conference paper [9].

As reported earlier, circular shaped micromixer showing the least concentration variance at the outlet. This was the most effective one among other models when the two electrode pairs were used [9].

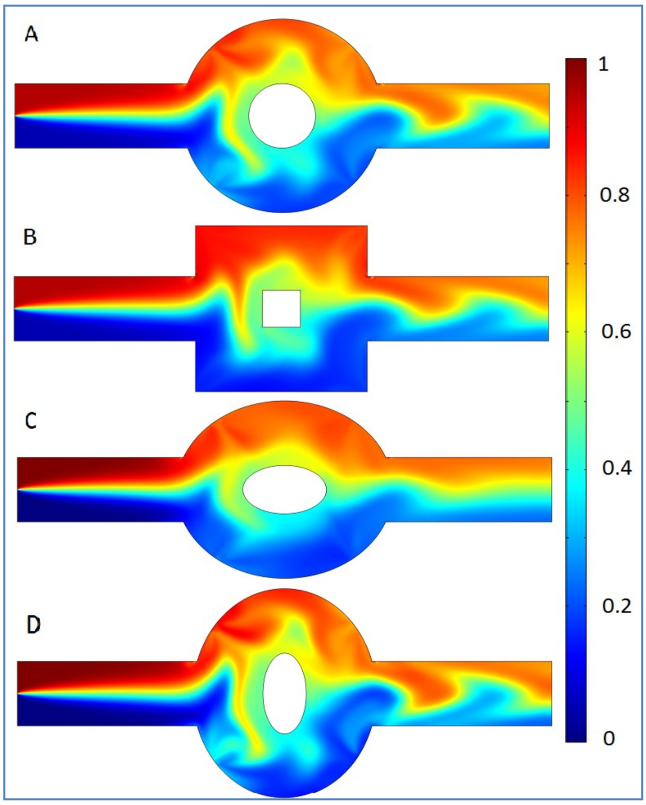

Fig. 2- Surface Concentration contours at time 0.27s with two electrode pairs for each shape: (A) circular, (B) square, (C) elliptic-I and (D) elliptic-II

As shown in [Fig-2], surface concentration distribution was seen to be significant in case of model D at the instant of 0.27 sec,. The upper left electrode in model D was found to be affecting more for uniform concentration distribution. From visual observation, yellowish narrow cone-like shape is extending longer in model D than model A. The corresponding concentration variance depicts more uniform distribution of species concentration.

Velocity Contours and Velocity Vectors

As shown in [Fig-3], velocity vectors showed the ionic fluid flow direction in various microchannels. Note that the logarithmic length of the arrows is chosen for to make velocity magnitudes proportional compared to the actual model sizes. The value in the Range quotient field (default: 100) determines the ratio between the smallest and largest values in the range of values for the logarithmic arrow length.

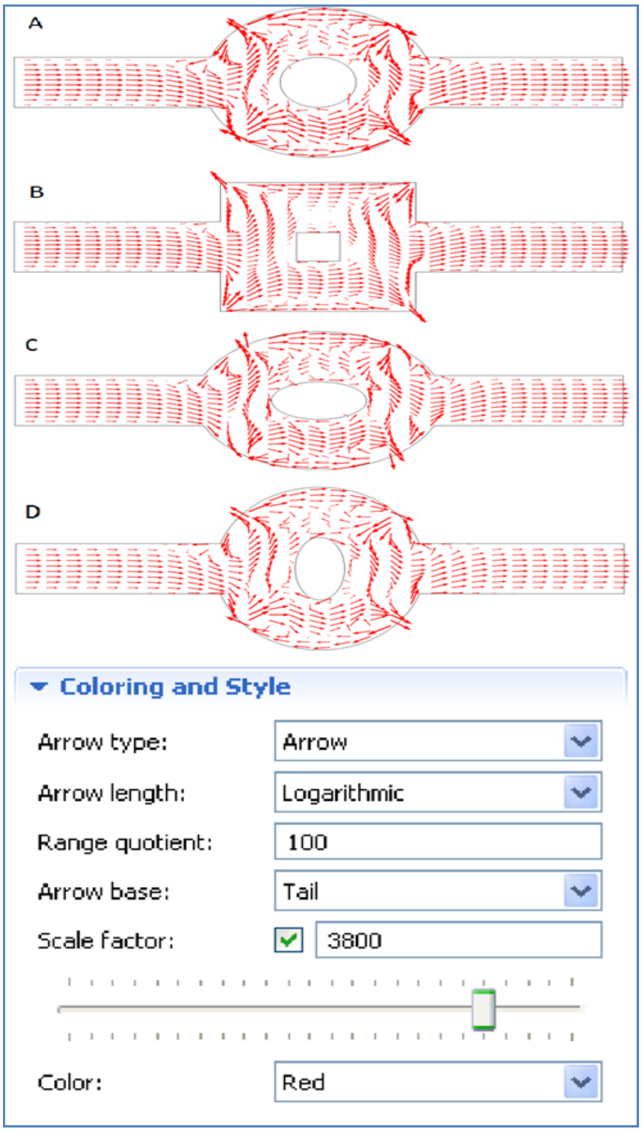

Fig. 3- Velocity vectors at time 0.27s with two electrode pairs for (A) circular, (B) square, (C) elliptic-I and (D) elliptic-II. Arrow lengths are logarithmically scaled to a range quotient of 100 and scaled to a factor of 3800 for models 'A &D' and to a factor of 4500 for models 'B & C'.

As shown in [Fig-4], velocity contours showed the ionic fluid flow distribution based on the velocity magnitudes in various microchannels. For the given micromixer models, the maximum velocity reached beyond the dark red colored contours at 0.27 sec for circular(A), square(B), elliptic-I(C) and elliptic-II(D). They were recorded 5.8255 mm/s, 4.8611 mm/s, 5.0482 mm/s and 5.5973 mm/s respectively. The lowest velocity of 3.822E-17 mm/s was found to be in square shaped micro mixer model.

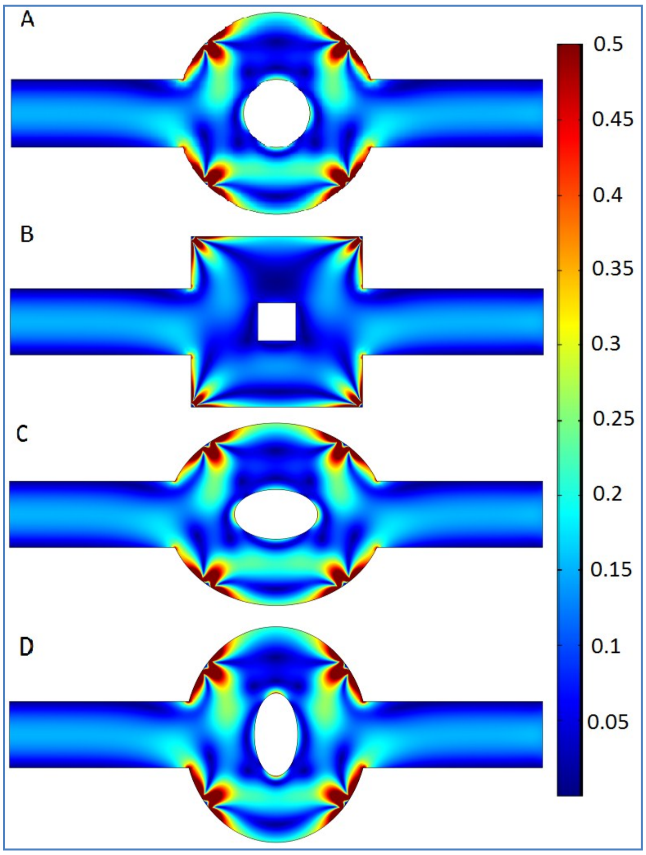

Fig. 4- Velocity contours capped up to 0.5 mm/s at time 0.27s with two electrode pairs for (A) circular, (B) square, (C) elliptic-I and (D) elliptic-II

This article presents our work as the continuation of our previously published conference paper [9]. Similarly, effects of m*ixing channel width, and electrode pairs* in concentration distribution and transient analysis in concentration distribution in microfluidic electroosmotic mixer can also be analyzed. This will be discussed in our future publications.

Conclusions and Recommendations

Our previous conference paper and the current study demonstrated the electro osmotic mixing is dependent on the electrode pairs [9]. Shape and size of the mixing channel also affects the effectiveness of mixing process. Circular mixer was found to be the most effective micromixer model and while using four electrode pairs. Though the fluid vortices were formed due to electric field, and perhaps the discontinuity in the channel geometry due to sharp corners make the stretching and folding of material lines unavailable to the non-concentrated species for the diffusive mixing for square shaped mixers. Magnetohydrodynamic (MHD) and electrokinetic (EK) flow in microfluidic chips has also been widely reported earlier. The proper utilization of MHD and EK effects along with other mixing parameters would be our future investigation for the development of a better lab-on-a-chip [9-16].

List of Abbreviations

DNA	Deoxyribonucleic acid
S	Concentration Variance
y	Coordinate axis in vertical direction
c	Concentration of the fluid at a given node
$\bar{c}$	Avg. concentration of fluid at a given boundary
dy	Elemental length in y-axis
μm	Micro meter
mol/m^3	Mole per meter cube
m	Meter
v	Velocity
V	Voltage
S/m	Siemens per meter
Hz	Hertz, cycles per second
ρ	Density of fluid
$\frac{\partial}{\partial t}$	Partial derivative with respect to time
∇	Del operator
P	Pressure
μ	Dynamic viscosity
ρ_e	Charge density
E	Electric field intensity
U_{slip}	Slip velocity
ε	Permittivity of the medium
ζ	Zeta potential
E_x	Electric field intensity at x-direction

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