Finite element modeling of acoustic streaming in SAW devices

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Abstract:

Fluid motion induced from high intensity sound waves is called acoustic streaming. SAW devices used in biological species detection suffer from fouling that results from binding of non-specific protein molecules to the device surface. The acoustic streaming phenomenon can be used to remove these non-specifically bound proteins to allow reuse of SAW devices. A finite element model of acoustic streaming phenomenon is presented in this work.

2-D FE models of SAW device based on YZ-LiNbO3 with a liquid loading are modeled. Solid domain based on a micron-sized piezoelectric substrate with dimensions (1600μm propagation length x 500μm depth) was simulated to gain insights into the acoustic streaming in SAW devices. Two IDT finger pairs in each port with periodicity of 34.87 μm were defined at the surface of Y-cut, Z-propagating LiNbO3 substrate. The IDT fingers were modeled as mass-less conductors and represented by a set of nodes coupled by voltage degrees of freedom (DOF). Fluid domain is modeled as an incompressible, viscous, and Newtonian using the Navier-Stokes equation. The incompatibility of the Lagrangian frame of reference for solid modeling and Eulerian frame of reference for the fluid is overcome by using the arbitrary Lagrangian-Eulerian (ALE) method where the mesh is constantly updated without modifying the mesh topology. To account for the fluid-solid interaction, an interface is defined across which displacements are transferred from solid to fluid and pressure from fluid to solid. The fluid mesh is continuously updated as the piezoelectric substrate undergoes deformation. The Standard k-ε Model is used to study flow in the turbulent regime. The structure was simulated for a total of 100 nanoseconds (ns), with a time step of 1 ns. The excitation of the piezoelectric solid was provided by applying an AC voltage (with varying peak value and frequency of 100 MHz) on the transmitter IDT fingers.

The above models are utilized to investigate methods for increasing induced acoustic streaming velocity while minimizing the effect on antibody sensing layer in immuno-SAW sensors. Parameters studied in this model include voltage intensity, and fluid viscosity. The transient solutions generated from the model are used to predict trends in acoustic streaming velocity.

1. Introduction

Fluid motion induced from high intensity sound waves is called acoustic streaming[1]. Surface acoustic waves propagating on the surface of a piezoelectric device can be used to induce acoustic streaming within the fluid. The streaming phenomenon finds applications in various processes ranging from mixing, surface reactions, sonic cleaning to biological detection[2] amongst several others.

SAW devices used in biological species detection suffer from fouling that results from binding of non-specific protein molecules to the device surface. The acoustic streaming phenomenon can be used to remove these non-specifically bound proteins to allow reuse of SAW devices. The generated sound fields cause tangential motion along the inter-phase boundaries. These motions exert steady viscous stress on boundaries where the circulation occurs. Although these stresses are not large, they are still significant enough to remove loosely bound material on the surface of the device. Understanding the fluid dynamics in

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such a system is useful for efficient removal of non-specifically bound proteins. Towards this end, we focus on how acoustic streaming transforms into a velocity field profile near the interface region of the piezoelectric substrate and the fluid loading.

Surface acoustic waves can be generated by the application of an alternating voltage signal to interdigital transducers (IDT) patterned on a piezoelectric substrate. The IDT geometry dictates the wavelength of the excited wave. The amplitudes of the SAW depend on the applied voltage input, and are typically in the nanometer range. SAW such as Rayleigh waves have a displacement component normal to the propagation direction. When in contact with a liquid, they tend to couple strongly and leak ultrasonic power into the fluid in the form of acoustic wave called as Leaky SAW. The leaky SAW decays exponentially with distance from the source. The SAW interaction creates a net pressure gradient in the direction of sound propagation in fluid which leads to an internal, acoustically induced streaming phenomenon. Experimentally, the resulting flow profiles can be captured using various techniques. Flow visualization employing a dye solution and a fluorescence video microscope has been carried out by Kondoh and Shiokawa[3]. On the other hand, Guttenberg et al. used fluorescent correlation microscopy (FCS) where movement of fluorescent particles is evaluated at the focal point of confocal microscope using time autocorrelation of the intensity fluctuations[4]. A velocity map can be generated by successive measurements at different positions inside the fluidic device.

Computational techniques such as finite element (FE) present an alternative to the experiments and can be used for more precise calculation of the flow field and velocity. Most of the previous theoretical investigations were based on methods such as Campbell-Jones or perturbational techniques and include many simplifying approximations[5-8]. These methods are typically used to study acoustic streaming in simplified geometries. FE models developed so far have been mostly limited to solve the fluid domain[9] motion where the solid motion is superimposed as a boundary condition. In order to capture the dynamics of fluid-solid interaction, the equations of motion for the fluid elements must be solved in conjunction with the acousto-electric equations for the motion of the solid. FE models involving coupling of fluid and solid domains has been carried out using acoustic elements for modeling the fluid region. However, these models solve only the simplified Navier-Stokes equation for the pressure field in the fluid and ignore the viscous dissipation. Uniform mean density and mean pressure are assumed, with the pressure solution being the deviation from the mean pressure, not the absolute pressure. The application of these models is limited to the study of wave damping.

A coupled field analysis takes into account the interaction between two or more disciplines of engineering. For example, a piezoelectric analysis of SAW device involves interaction between structural and electric fields. Other examples include thermal-stress analysis for bimetallic actuators, magneto-structural analysis of electromagnetic actuators, fluid-structure analysis for fluid flow considerations and problems that involve complex interaction of the structural and electrical fields with the flow field. The last one represents one of the most complex analyses of micro-systems. An example of the analysis of electric-structure-fluid coupled micro-system is that of fluid loading on top of the SAW biosensor device.

In the present case, the problem of interest requires us to model fluid motion which can be accomplished using CFD elements which solves the generalized Navier-Stokes equation. To the best of our knowledge, no FE model involving coupled field analysis of fluid-piezoelectric SAW device is available in literature. In the present work, FE models involving fluid-piezoelectric interaction are developed to study flow profiles on the interface region in a SAW biosensor device. The above models are utilized to investigate methods for increasing induced acoustic streaming velocity while minimizing the effect on antibody sensing layer in immuno-SAW sensors. Parameters studied in this model include voltage intensity, frequency, fluid density, and viscosity. The transient solutions generated from the model are used to predict trends in acoustic streaming velocity. In addition to the above parameters, the effect of various interdigital transducer (IDT) geometry/design on the streaming velocity is also investigated. Comparisons of model predicted trends with experimental data on the removal of non-specifically bound proteins from the sensing layers will also be presented.

2. Computational details:

Solid domain

A system of four coupled wave equations for the electric potential and the three component of displacement in piezoelectric materials are solved for the piezoelectric substrate or the solid domain[10]:

$$-\rho \frac{\partial^2 u_i}{\partial t^2} + c^E_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l} + e_{kij} \frac{\partial^2 \phi}{\partial x_k \partial x_j} = 0 \qquad \textbf{(2.1)}$$

$$e_{ikl} \frac{\partial^2 u_k}{\partial x_i \partial x_l} - \varepsilon^S_{ik} \frac{\partial^2 \phi}{\partial x_i \partial x_j} = 0 \qquad \textbf{(2.2)}$$

These coupled wave equations can be discretized and solved for generating displacement profiles and voltages at each element/nodes. The piezoelectric material displacements obtained from the above equations are applied to the fluid domain.

Fluid domain

Fluid is modeled as an incompressible, viscous, Newtonian fluid using the Navier-Stokes and continuity equation in the Eulerian frame of reference given below:

$$\rho\left(\frac{\partial v_f}{\partial t}\right) + v_f \cdot \nabla v_f + \nabla P - 2\eta \nabla \cdot D = 0 \qquad \textbf{(2.3)}$$

$$\nabla \cdot v_f = 0 \qquad \textbf{(2.4)}$$

Here, v_f, P, ρ and η denote the fluid velocity, pressure, density, and viscosity, respectively. D is the rate of deformation tensor given by

$$D = \frac{1}{2}\left(\nabla v_f + (\nabla v_f)^T\right) \qquad \textbf{(2.5)}$$

Fluid-solid interaction

The equations of motion described above were based on an Eulerian (fixed) frame of reference. The governing equations may also be formulated in a Lagrangian frame of reference, i.e. the reference frame moves with the fluid particles. Both formulations have their advantages and disadvantages. With the Eulerian framework it is not straightforward to solve problems involving moving boundaries or deforming domains. While such problems are more suitable for a Lagrangian framework, in practice the mesh distortions can be quite severe leading to mesh entanglement and other inaccuracies. A pragmatic way around this problem is to move the mesh independent of the fluid particles in such a way as to minimize the distortions.

The incompatibility of the Lagrangian frame of reference for solid modeling and Eulerian frame of reference for the fluid is overcome by using the arbitrary Lagrangian-Eulerian (ALE) method where the mesh is constantly updated to track the boundary motion/domain deformation without modifying the mesh topology. To account for the fluid-solid interaction, an interface is defined across which displacements are transferred from solid to fluid and pressure from fluid to solid. The fluid mesh is continuously updated as the piezoelectric substrate undergoes deformation.

In the ALE framework, the fluid equation of motion can be written as[11]:

$$\rho\left(\frac{\partial v_f}{\partial t}\right)+(v_f-w)\cdot\nabla v_f+\nabla P-2\eta\nabla\cdot D=0\ ; \qquad \mathbf{(2.6)}$$

w is the grid velocity such that $w \neq v_f \neq 0$.

The coupling conditions for the interface between the fluid and the solid region are the kinematics and equilibrium condition. The kinematic equation is the no-slip condition, i.e. the continuity of velocity:

$$v_f = v_s = \frac{\partial u}{\partial t} \qquad \mathbf{(2.7)}$$

and the equilibrium condition is the interface continuity in tractions replaced by continuity of stresses:

$$\sigma_{ij}^S n_j^S + \sigma_{ij}^f n_j^f = 0 \qquad \mathbf{(2.8)}$$

where n_j^S is the outward normal to the solid at the solid-liquid interface in the deformed configuration, so that $n_j^S = -n_j^f$ (indices *i* and *j* define directions of components according to axes of the applied 2-D coordinate system). The above equations are represented in terms of partial differential equations which are discretized using finite element technique[12].

3. Model formulation

A finite element model of acoustic streaming phenomenon is presented in this work. Rayleigh wave propagation on a SAW device represents a plane wave problem. Hence, 2-D FE models of SAW device based on YZ-LiNbO3 with a liquid loading are modeled.

Solid-domain

A micron-sized piezoelectric substrate with dimensions (800µm propagation length x 500µm depth) was simulated to gain insights into the acoustic streaming in SAW devices. Three IDT finger pairs for the input port were defined at the surface of Y-cut, Z-propagating LiNbO3 substrate. The fingers were defined with periodicity of 34.87 µm. The IDT fingers were modeled as mass-less conductors and represented by a set of nodes coupled by voltage degrees of freedom (DOF). A total of approx. 80,000 elements (more than 100000 nodes) were generated. The model was created to ensure higher node density at the surface and throughout the middle of the device to study the different modes of surface acoustic waves and the use of 8-node coupled field (solid) elements with 3 DOF ensured the same. Two DOF's provided the displacements in the longitudinal (x), and the normal (y) directions and a third for the voltage.

Fluid domain

4-node quadrilateral fluid elements are used to model the transient system involving fluid region. The fluid properties of water were used in the simulations. The velocities are obtained from the conservation of momentum principle, and the pressure is obtained from the mass conservation principle. The fluid region with dimensions (800µm length x 100µm height) was modeled as an infinite reservoir by applying pressure P=0 on the upper fluid surface in Fig. 1. The standard k-ε Model is used to study flow in the turbulent regime.

Structure excitation

The structure was simulated for a total of 100 nanoseconds (ns), with a time step of 0.5 ns. The excitation of the piezoelectric solid was provided by applying an AC voltage (with varying peak values and frequency of 100 MHz) on the transmitter IDT fingers.

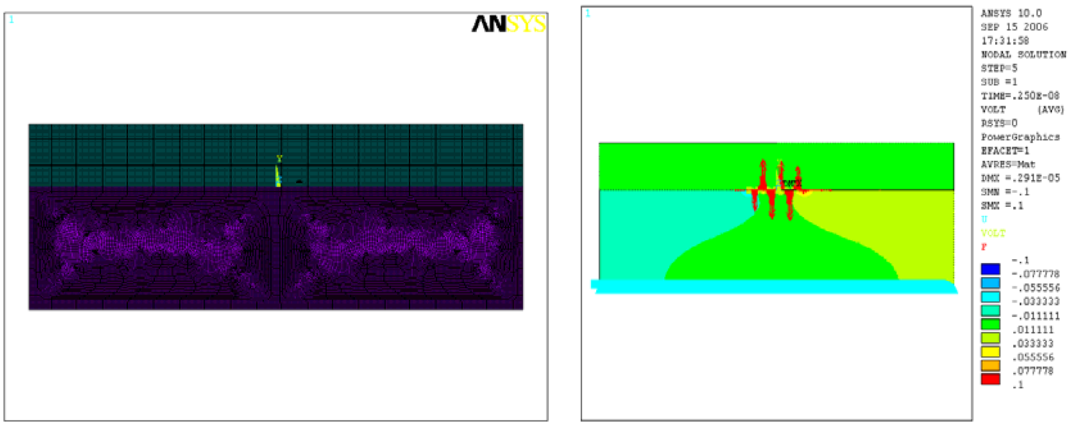

Figure 1. (a) Finite element model of liquid loading on a SAW device. (a) Contour plot showing the direction of movement of IDT fingers located at the center on the surface of the piezoelectric device at t=2.5 ns.

4. Results and discussion

The following sections discuss the wave mode conversions that results from the imposed fluid loading as well as the flow profiles of the induced fluid motion. The effect of various design parameters on the streaming velocity profiles and pressure is also presented.

i. Rayleigh wave Mode conversion

When the surface acoustic wave propagation surface comes in contact with a liquid medium, mode conversion from Rayleigh to leaky SAW occurs. This leaky SAW propagates along the boundary and excites longitudinal wave into the fluid at Rayleigh angle (θ) given by:

$$\theta = Sin^{-1}\left(\frac{v_w}{v_R}\right)$$

v_w and v_R are the wave velocities in the liquid and piezoelectric medium. The ultrasonic radiation mechanism is shown in Fig. 2.

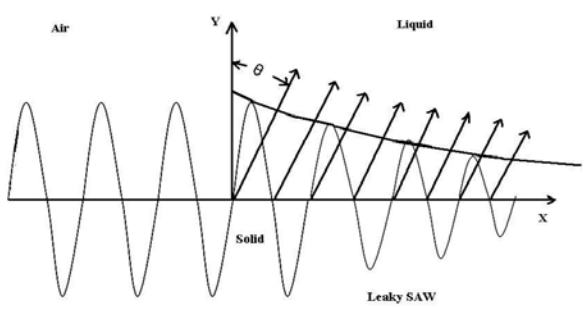

Figure 2. Ultrasonic radiation into the fluid medium.

The generated longitudinal sound waves in the fluid medium are attenuated by the viscosity along its transmission through the medium. The displacement profile along the fluid film thickness for an applied voltage of 1V is shown in Fig. 3. It can be seen that the mode conversion from Rayleigh to Leaky SAW leads to an exponential decay in the fluid. The extent of the decay is dictated by the applied input voltage as well as the viscous dissipation encountered by the longitudinal wave in the fluid medium. The leaky surface wave also decays along the propagation length as shown by the displacement contours in Fig 4.

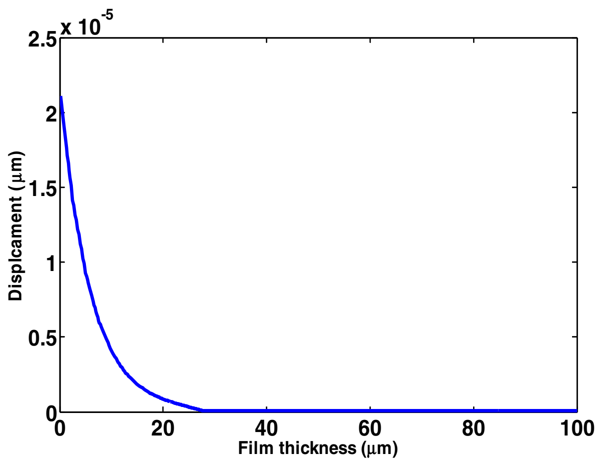

Figure 3. Displacement profile along the film thickness induced as a result of leakage of ultrasonic SAW power into the fluid. The exponential decay with distance from the source is similar to that of Leaky SAW.

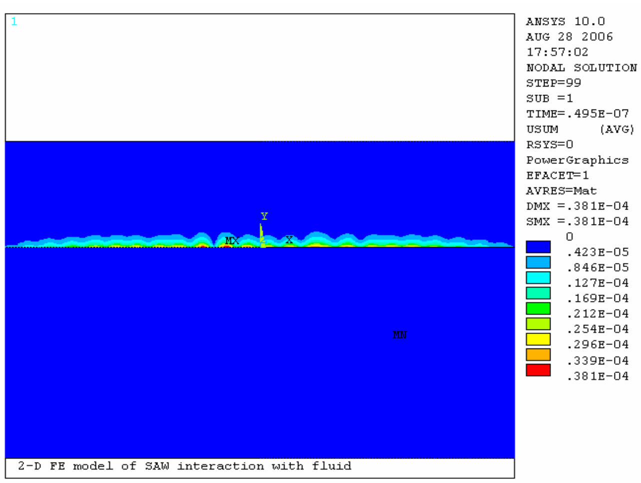

Figure 4. Displacement contours in fluid region for an applied AC peak voltage of 1 V. The wave decays with distance from the IDT fingers located at the center of the device. The displacements in the solid have been suppressed for clarity.

ii. Fluid Motion (displacement contours)

If the intensity of the longitudinal waves propagating through the fluid is high enough, then the attenuation results in a net pressure gradient along the propagation direction of the wave. The induced gradient causes a flow in the fluid. This conversion of attenuated sound wave into a steady flow represents a nonlinear effect termed as acoustic streaming. The streaming effect that results from mode conversion is much stronger than that induced from a spatially constant amplitude plane wave[12].

The fluid motion induced by the IDTs at any given instant of time is shown in Fig. 5. The fluid is expelled by the transducers to the top and flows back to the IDT regions from the bottom and top. Depending on the extent of the viscous damping, the flow velocity decays rapidly with distance from the IDT.

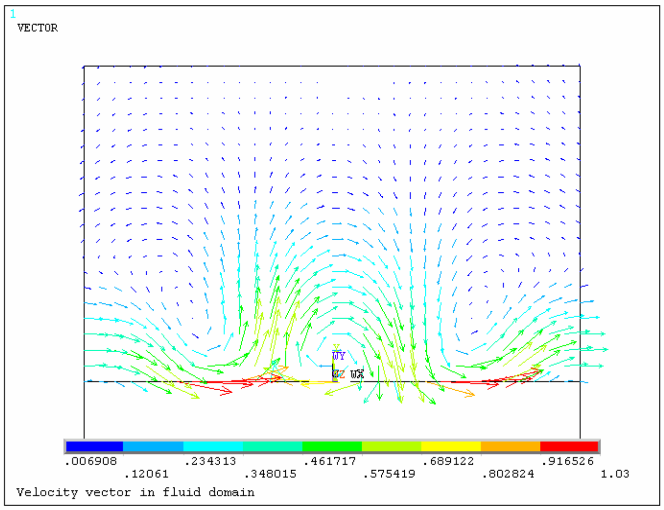

Figure 5. Velocity vector plot showing fluid recirculation over the IDT region.

It can the seen that the induced velocities are typically in microns/sec. The maximum velocity occurs at the layer closest to the piezoelectric surface. The recirculation patterns resulting from the wave motion gives rise to eddy formation. With increasing time, these eddies rise through the fluid and break into smaller ones, thereby dissipating their energy while new ones are created at the interface. Thus, the generated sound fields cause tangential motion along the inter-phase boundaries. These motions exert steady viscous stress on boundaries where the circulation occurs as shown in Fig. 6. Although these stresses are not large, they are still significant enough to remove loosely bound material on the surface of the device. Our simulation results show that the extent of recirculation decreases with increasing distance from the IDTs. It can therefore be seen from Fig. 6 that the generated shear stresses at the device surface also decay rapidly with distance from the IDT fingers. Optimization of design parameters such as fluid density, viscosity and applied voltage amplitude and frequency which could help generate sufficient shear stresses along the entire delay path (typically 100λ) thereby facilitating removal of nonspecifically bound proteins is required. The subsequent sections discuss the effect of some of the above mentioned parameters on the induced streaming velocity.

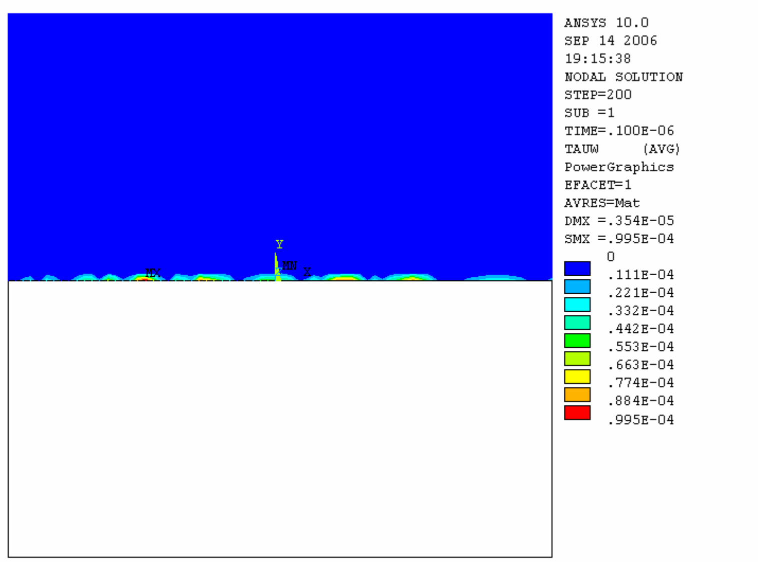

Figure 6. Shear stresses (MPa) generated as a result of the recirculation at the surface of the SAW device. The applied input voltage was 0.1 V and the fluid viscosity was 10 cP.

iii. Streaming velocity

The finite element model of SAW streaming presented here is utilized for determining steady state streaming velocity profiles associated with a given transducer geometry and input acoustic pulse. Experimentally, the observed streaming velocities are smaller than 20 mm/s for the loading conditions simulated in the present work and, hence for a fluid film thickness of 100 microns, the flow is characterized by Reynolds number smaller than 1. Hence the flow is completely laminar.

Effect of voltage intensity

The effect of varying input voltage intensity on streaming velocities is shown in Fig. 7.The fluid velocities are obtained at different positions along the fluid film thickness normal to the piezoelectric substrate. It can be seen that the highest velocities are attained in the region closer to the piezoelectric device. The maximum flow velocity varies from approximately 15 µm/s to 15 mm/s, depending on the applied input voltage. The velocities decrease rapidly with increasing distance from the IDT surface. Most of the fluid motion is confined to within the first few layers (approx. 20 microns).

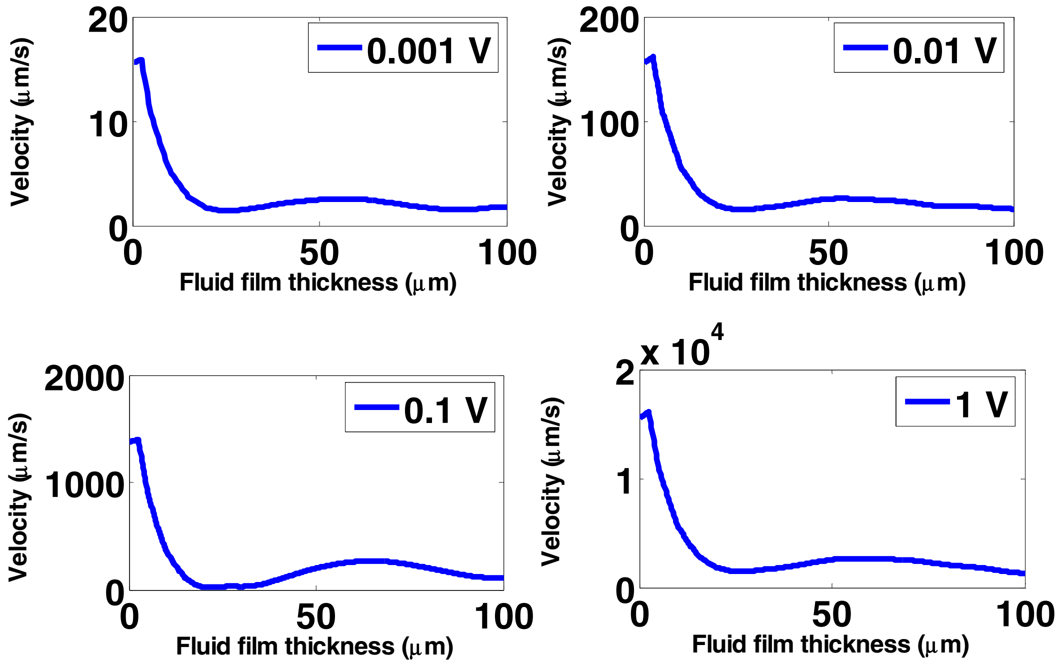

Figure 7. Simulated streaming velocity profiles along the thickness of the fluid film. The applied input voltage was varied from 1 mV to 1 V. The streaming velocity varies approximately linearly with the applied input voltage.

As the distance increases along the propagation direction, the extent of induced fluid motion and consequently the fluid velocity decrease. The extent of damping is dictated by the shear viscosity of the fluid. The simulated data at any particular fluid location can be fitted to a linear relationship of the velocity on the applied voltage.

The effect of other parameters such as fluid viscosity, fluid density and applied voltage frequency on the induced streaming velocity is currently under investigation. The trends in the velocity profiles would be used to identify parameters which would help maximize removal of non-specifically bound proteins while minimizing the effect on the antibody sensing layer.

5. Conclusions

2-D finite element models of a liquid loading on top of a piezoelectric SAW device were developed. The interaction of generated Rayleigh wave on the SAW device surface with the liquid loading was investigated. The SAW interaction with fluid leads to an internal acoustically induced streaming and results in a mode conversion to a longitudinal wave called as Leaky SAW which decays exponentially with distance in the fluid. The velocity vector field shows recirculation patterns in the fluid region resulting from the out of phase motion of the IDT fingers. The fluid recirculation exerts steady viscous stresses on the inter-phase boundaries which can be used for the removal of non-specifically bound proteins. The extent of recirculation and therefore the induced stresses decrease with distance from the IDT fingers. Optimization of parameters which can maximize the streaming and cause removal of unwanted proteins along the entire delay path is required.

One of the parameters i.e. input voltage amplitude was varied and it was found that that the induced streaming velocity varies linearly with the applied input voltage. Therefore the higher the applied voltage the greater would be the extent of cleaning. This agrees well with the experimental observations. The study of effect of other parameters such as fluid density, viscosity and input voltage frequency on acoustic streaming is currently underway. It is expected that the model generated trends would serve as guidelines for subsequent experimental investigation.

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