Numerical simulation of cell stirring and separation in a micro droplet using surface acoustic wave-driven flow

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Abstract: Flow generation techniques using surface acoustic wave (SAW) have been developed. This technique is useful for the mixing/separation of particles in a small droplet and can be applied for the laboratory testing with extremely small amount of specimen. In this study, a hemispherical shaped micro water droplet with a volume of 30 μL was modeled and the SAW-driven flow in the droplet was numerically calculated. The calculation results show that a vortex generated around the SAW irradiation site moves toward the droplet center and it derives upward flow. The particles with the same degree as the density of water follows the flow field in the droplet and eventually pile on the peripheral area. The particles with high density moves toward the droplet center along the substrate surface and accumulate at the central area. The feasibility of cell separation was confirmed from the numerical simulations.

Keywords: Surface Acoustic Wave (SAW), Cell Mixing/Separation, Micro Droplet, Computational Fluid Dynamics (CFD)

1. Introduction

A surface acoustic wave (SAW) is an acoustic wave and propagates along the surface of an elastic body. SAW can be continuously excited by inputting alternating current signal between the comb-shaped electrodes of an interdigital transducer (IDT) deposited on top of a piezoelectric substrate at a resonant frequency, and it propagates on the substrate surface. In contrast, IDTs is also used to convert acoustic waves to electrical signals. These devices are called as SAW devices and widely used as filters, oscillators and transformers in electric circuits.

In recent years, SAW has been applied to drive fluid in microfluidic devices. An acoustic wave propagating through a liquid loses its energy because of viscous wave damping and generate acoustic streaming flow in the fluid. The acoustic streaming flow is used for mixing in a droplet, translocation of a droplet nebulization of liquid, pumping of fluid, etc.

In this study, SAW-driven flows in a micro water droplet and column model were numerically calculated to investigate the flow generation process. And also, we investigated the applications of the acoustic streaming flow to cell stirring and mixing through numerical simulation.

2. Methods

2.1 Computational model

Two types of micro water droplets were modeled using three dimensional computer-aided design (3D CAD) software. One is a model of a droplet placed on a substrate. The shape was approximated as a hemisphere with a volume of 30 μL and a radius of 2.43 mm. The other is a model of a water column formed between two substrates placed in horizontally parallel. The water column model was approximated as a cylinder with a volume of 90 μL, a diameter of 4.86 mm and a height of 4.86 mm.

Cartesian coordinate systems were defined as shown in Fig. 1. The origins were put at the front tips of the droplet and column on the bottom substrates. The z-x plane was placed on the bottom substrate and x axis was set toward the SAW propagation direction. The y axis was set toward vertically upward. The fluid domains of these models were discretized by unstructured meshes.

2.2 Flow calculation

SAW is assumed to be irradiated from the front side of the water droplet and column models on each bottom substrate and also from the back side of the column model on the upper substrate as shown in Fig. 1. The SAW irradiation band with a width of 2 mm are offset 1.2 mm from the model center. In this study, a SAW device on a LiNbO3 substrate with a resonant frequency of $f = 62$ MHz was assumed.

The flow in the models were calculated by solving Navier-Stokes equation and equation of continuity (Eq.(1) and (2)).

$$\frac{\partial U_j}{\partial t} + (U_j \cdot \nabla) U_j = F_j - \frac{1}{\rho} \nabla p + \nu \nabla^2 U_j$$

(1)

$$\nabla \cdot U_j = 0$$

(2)

In Eq. (1) and (2), $U_j$ is flow velocity, $t$ is time, $F_j$ is external body
force \( \rho \) is density, \( p \) is pressure and \( v \) is kinematic viscosity. The external force caused by SAW irradiation is described as

\[
F_x = \rho(1 + \alpha^2)A^2\omega^2k_0\exp(-2(k_0x + \alpha k_0y)) \tag{3}
\]

\[
F_y = \rho(1 + \alpha^2)A^2\omega^2k_0\exp(-2(k_0y + \alpha k_0x)) \tag{4}
\]

where \( \alpha \) is attenuation coefficient 2.47, \( A \) is amplitude of SAW, \( \omega \) is angular velocity \((2\pi f)\), and \( k_0 \) is the wave number of leaky SAW 2768 m\(^{-1}\). The SAW-induced force was substituted to the external force term of Navier-Stokes equation. These equations were numerically calculated using a computational fluid dynamics (CFD) software (ANSYS-CFX, ANSYS, Inc.). The fluid is assumed to be water at a temperature of 25 °C. The density and dynamic viscosity were set to 997 kg/m\(^3\) and 8.899×10\(^{-4}\) Pas, respectively. A non-slip condition was applied to the solid-liquid interface and a slip condition was applied to the gas-liquid interface. The deformation of the interfaces was assumed to be negligible because of the low SAW power. Assuming that the flow in water droplet models was completely stationary at the initial time step of the calculation \((t = 0)\), the process of flow generation was calculated.

2.3 Particle tracking

The trajectories of particles in the water droplet and column models are calculated by considering viscous and buoyancy forces acting on the particles. The equation of particle motion is expressed as Eq. (3).

\[
m_p \frac{dU_p}{dt} = F_D + F_B \tag{3}
\]

where subscript \( p \) means particle, \( m \) is mass, \( U \) is velocity, and \( t \) is time. \( F_D \) and \( F_B \), meaning drag force and buoyancy force, are described as Eq. (4) and (5), respectively.

\[
F_D = \frac{1}{2}C_D \rho_f S_f |U_f - U_p| |U_f - U_p| \tag{4}
\]

\[
F_B = \frac{\pi}{6}d_p^3(\rho_p - \rho_f)g \tag{5}
\]

where subscript \( f \) means fluid, \( C_D \) is drag coefficient, \( \rho \) is density, \( S_f \) is effective cross sectional area, \( d \) is particle diameter, and \( g \) is gravitational acceleration. Red blood cells (RBCs), white blood cells (WBCs) and iron powder are modeled as spherical particles. The parameters of these particles are shown in Table 1. The particle injecting points are placed in the plane parallel to each substrate.

3. Results and discussion

3.1 SAW-induced flow field

The SAW-induced flow in a micro water droplet are drawn in Fig. 2 as streamlines starting from the plane 0.1 mm upper from bottom substrate. The SAW amplitude is set to 3.35 Å. Just after the starting of SAW irradiation, flow is slightly generated around the bottom substrate. Vertical upward flow is generated around \( t = 0.06 \) s. At \( t = 0.2 \) s, a vortex is formed around the SAW irradiation site and then it grows and moves toward the droplet center. At \( t = 1.5 \) s, the vortex almost reaches to steady state. The top views showing the flow in droplet indicate that the vortex core locates slightly to the SAW-irradiation side at steady state. On the droplet surface, oblique upward flow is generated at front side and overall circumferential flow is formed as show in Fig. 3.

The SAW-induced flow in a micro water column are drawn in Fig. 4 as streamlines starting from the plane 0.1 mm upper and lower from lower and upper substrates, respectively. The SAW
amplitude is set to 3.35 Å. Two small vortices are formed around the SAW irradiation site on the upper and bottom substrates and they transition to upward and downward vortex flows from the lower and upper substrates, respectively. The rotational directions of the vortices are same. These are combined around $t = 0.5$ s and then the combined vortex core is aligned to the column center axis. The flow field almost reaches to steady state until 1.5 s after the starting of SAW irradiation ($t = 1.5$ s). On the water column surface, overall circumferential flow is generated at steady state as shown in Fig. 5.

3.2 Particle trajectories

The particle trajectories in SAW-induced flow field were calculated. The particle trajectories in a micro water droplet model is shown in Fig. 6. The RBC and WBC particles, which have almost same density as water, follows the flow field in the droplet at the SAW amplitude of 2.0 Å, i.e. particles are moved along the bottom surface toward the droplet center, turned vertically upward following the center vortex flow and then turned around in the droplet. Therefore, this system is suitable for cell stirring. After

Fig. 4 SAW-induced flow in a micro water column model (front view).

Fig. 5 SAW-induced flow on a surface of a micro water column model.

Fig. 6 Particle trajectories in a micro water droplet model.
stopping the SAW irradiation, RBC and WBC particles pile on the peripheral area. In contrast, the iron powder particles with high density are moved toward the droplet center along the substrate surface by SAW-induced flow and accumulate at the central area at the SAW amplitude of 5.0 Å. Separation of cells and high density particles can be achieved by this system.

The particle trajectories in a micro water column model is shown in Fig. 7. The RBC particles follows the rotational flow generated in the column model at the SAW amplitude of 2.0 Å. Therefore, this system would enable three-dimensional-stirred suspension culture without rotating blades.

4. Conclusions

The SAW-driven flows in a micro water droplet and column model were numerically calculated and the flow generation process was revealed. Furthermore, the applications of this system to cell stirring and mixing were investigated and the feasibility was confirmed.

Reference