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Numerical Analysis of Particle Sorting by Acoustic Waves in Microfluidics

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Abstract: Microfluidics holds great promise for manipulating particles. This field is particularly important for biomedical, lab-on-chip environmental, and chemical analysis. Several techniques have been adopted and developed to increase the efficiency of particle sorting. These methods include fluorescence-activated cell sorting, electrophoresis, gravitational, optical, and magnetospheric sorting. This article conducts a comprehensive literature review to understand the methodologies implemented in recent years. This paper aims to investigate and model particle separation dynamics in a microfluidic channel utilizing the piezoelectric transducer. Specifically, it seeks to optimize separation efficiency by analyzing the influence of the system's resonant frequency on manipulating and sorting particles within the microfluidic environment. The other goal is to characterize the effects of different parameters, such as flow rate, water content, and resonant wave frequency. The study used numerical methods to avoid an expensive experimental setup. The simulation revealed that particles exposed to acoustic waves undergo separation across the width of the channel. It is also observed that important parameters like flow rates, frequency, and diameter of the particles influence the sorting efficiency. Thus, this paper will advance our theoretical knowledge of the interactions between acoustic waves and particles, which can be a reference to the design of advanced microfluidic systems for future applications.

Keywords: Microchannel, piezoelectric transducer, acoustic energy, particle sorting

Introduction: Particle sorting is important because it allows precise identification and isolation of specific particles from a complex mixture. This field is particularly important in biosensing, drug delivery systems, genomics, and proteomics [1]. For instance, in biomedical and biological research, the capability to isolate specific particles and cells from a mixed environment is regarded as a crucial technique for studying individual cells or particles. Therefore, this technology has led to significant breakthroughs in cell biology, offering the potential to assess a patient's health status accurately [2] The other applications can be fuel oil purification and pollution reduction since burning fossil fuel is responsible for emitting materials like CO, HC, and NOx [3]. The consequence of these emissions can have a tremendous negative impact on the environment, which causes global warming and climate change, leading developing countries like Bangladesh to suffer the most due to these unwanted pollutants [4]. Incorporating microfluidic particle sorting into fuel oil processes can target improving fuel quality and efficiency while reducing emissions.

This system can enable meticulous manipulation of flow dynamics, which can be customized to effectively remove particulate contaminants and unwanted chemical droplets from fuels. In general, microfluidics channels can utilize two types of sorting techniques; in the passive method, channel geometry and the flow field are used without considering any external energy, and in active sorting, the external field is implemented for better outcomes [5]. For particle sorting, microfluidic technology has significant advantages for the precise manipulation of micro and nanoparticles, and the separation of these particles based on ultrasonic standing waves has attracted much attention for its high efficiency and simplicity of structure [6]. In addition, PDMS (polydimethylsiloxane) based microfluidic devices ensure accurate sorting by their capacity to regulate characteristics like size, shape, and surface qualities. The patterned regions are also protected from oxygen plasma by controlling the dimensions of the PDMS stamp and by leaving the stem in place during the plasma treatment process [7]. They can also be easily integrated with imaging systems and sensors for automation and functionality. They are also economical because they need little in the way of reagents and samples. They have diverse applications in biology and medicine because of their compatibility with biological materials, making them a flexible and effective platform for particle sorting across various scientific fields provided by microfluidic devices. These channels can be fabricated by soft lithography, which allows the researcher to make complex devices affordably and simply [8]. The operation starts with fabricating a microchannel structure, which is patterned on a substrate, and the channel geometry is defined by selectively removing material via etching. Once the channel is replicated on PDMS and attached to the glass slide with piezo, the fluid from the syringe pump can be supplied, keeping the acoustic transducer switched on to agitate the particles, and the microscope observes the overall phenomenon.

Literature Review: The literature reveals a growing interest in piezoelectric transducers in conjunction with microfluidic channels for particle separation. Studies have developed to understand the intricate interplay between acoustic forces generated by the transducer and particle behavior within the microfluidic environment, offering insights into optimizing separation performance

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and device design for diverse applications. However, finding the resonance frequency is essential for utilizing the acoustic energy in microfluidics. S. M. Hagster et al. [9] employed micro-PIV analysis alongside images of transient particle movement to experimentally investigate acoustic radiation forces and acoustic streaming within microfluidic chambers. Their research conducted full-image micro-PIV studies of acoustic resonances in piezo-actuated, flat microfluidic chambers containing different tracer particles, allowing them to observe the particles' behavior in the acoustic field. Another work by Kyriacos Yiannacou and Veikko Sariola[10] proposed an adaptive control technique for the acoustic manipulation of individual and multiple particles within microfluidic chips. They mounted a piezoelectric transducer back of the glass microfluidic channel, and a machine vision algorithm was implemented to track the position of the particles. Their method is based on online machine learning of the acoustic fields. They found that controllers can manipulate particles even on the first attempt, and their performance improves in subsequent attempts. Cristian Brandi et al. [11] implemented a piezo transducer on the flow of polystyrene beads suspended solution to monitor the streamlines considering the sinusoidal and pulse actuation. They showed that similar voltage levels (a few volts) were required to produce significant fluid deflection by several degrees for numerical simulations and experimental observations. In both instances, the degree of fluid displacement appeared to correspond roughly to the magnitude of the applied voltage. Citsabehsan Devendran et al. [12] demonstrated how the acoustic radiation force (ARF) drives particles away from pressure antinodes positioned on either side of the pressure node. As a result, particles will either move toward the bottom of the channel at the center (the pressure node) or toward the edges of the fluid volume, depending on their primary location. Their results reveal the behavior of different-sized particles in the presence of acoustic streaming and ARF, and it suggests that acoustic streaming—a swirling motion caused by acoustic waves—is the main factor influencing the behavior of tiny particles, about 1 micrometer in size. However, larger particles—roughly 10 micrometers influenced by the Acoustic Radiation Force- go to desired areas**.** Therefore, their size is a major factor in identifying the main forces influencing the movement and behavior of the particles. A. Bakhtiari and C. J. Kähler [13] conducted comprehensive statistical analysis, including flow characterization through volumetric micro-PTV, high-frequency micro-PTV to observe flow field transitions, assessment of the system's particle trapping efficiency for various particle sizes using a proprietary algorithm, and examination of the z-axis distribution of both captured and escaped particles using volumetric micro-PTV. In this work, they ran the experiment at different frequencies and amplitudes for various-sized particles. They found that for a specific amplitude, 66 Vpp, and frequency of 33kHZ of the piezoelectric transducer for the designed channel, 10-micron particles emerged almost 100% successful compared to 5- and 15-micron particles. This study investigates how particles respond to acoustic, hydrodynamic, and electric forces in a fluidic environment. By simulating these forces, the study aims to improve particle sorting efficiency for applications like biomedical diagnostics and lab-on-chip technologies.

Governing Equation:

Achieving maximum efficiency requires careful consideration of frequency magnitude, and the applied frequency can be calculated as [15]

... …Eq.1

In this simulation, we used a single mode of resonance within the channel, so $n_x, n_z = 0$, and therefore, the resonance frequency becomes

$$
f_{0,1,0} = \frac{c_f}{2w} \tag{Eq.2}
$$

Here C_f is the sound's speed in the water. When a particle is present in an acoustic field, the incident waves on the particle scatter, causing acoustic radiation force causing the particle to move toward either the pressure nodes or antinodes. The direction of this movement depends on the sign of the acoustic contrast factor [6]. Additionally, a drag force arises due to the relative motion of the particle within the viscous fluid. This force opposes the particle's motion and is influenced by the viscosity of the surrounding medium.

Applying Newton's second law for force balance [13], we get-

$$
F_{drag} + F_{rad} = m \frac{d^2 r}{dt^2} \tag{Eq3}
$$

where m and **r** denote the mass and displacement of the particle, respectively. The particle radius r influences the drag force experienced by spherical particles moving at a velocity *Vp* through a fluid with a different velocity *Vf* and viscosity becomes [14]

$$
F_{drag} = -6\pi\eta a (V_p - v_f) \tag{Eq.4}
$$

Volume 04, Issue 02, 2024 Page 18

This equation considers the interaction between the particle and surrounding fluid, accounting for velocity, size, and fluid properties. The acoustic radiation force acting on a particle in a fluid under the influence of a sound field is typically given as follows [6]

$$
F = \frac{-p_{\Delta}^{2}vp_{\Delta}}{2\lambda}\varphi(k,\rho)\sin(2kx) \tag{Eq.5}
$$

$$
\phi(k,\rho) = \frac{(5\rho_{y-2}\rho_0)}{(5\rho_y + \rho_0)} - \frac{k_y}{k_0}
$$
 ...Eq.6

 $Pa=$ is the peak sound pressure, v_p is the volume of a particle

 $K_{p=}$ compressibility of particles, $\kappa_{0=}$ compressibility of water

 ρ_p and ρ_0 are the density of particles and water, respectively.

 Φ is the acoustic contrast factor. When $\Phi > 0$, the acoustic radiation force drives the particles to move toward the pressure node; when Φ < 0, the acoustic radiation force drives the particles to gather toward the pressure anti-node [6].

From the equations 3,4,5 and 6, we get,

$$
-6\pi\eta a \left(V_p - v_f\right) + \frac{-p_a^2 V p K_0}{2\lambda} \left(\frac{(5\rho_{p-2}\rho_o)}{(5\rho_p + \rho_o)} - \frac{k_p}{k_o}\right) \sin(2kx) = m \frac{d^2r}{dt^2}
$$
 ... Eq. 7

The discretized version, with the central difference method of Eq. 7

$$
-6\pi na \left(v_p - v_f\right) + \left(-\frac{p_d^2 v_p k}{2\lambda}\right) \left(\frac{(5\rho_{p-2}\rho_0)}{(5\rho_p + \rho_0)} - \frac{k_p}{k_0}\right) sin(2kx) = m \frac{r(t+\Delta t) - 2r(t) + r(t-\Delta t)}{\Delta t^2} \tag{1.50}
$$

Where $r(t + \Delta t)$, $r(t)$, $r(t - \Delta t)$ indicated positions at times $(t + \Delta t)$, t , and $(t - \Delta t)$, respectively.

Materials and Method: The simulation was carried out with MATLAB and the code is written based on Eq.8 to track the particles over time. The channel in this simulation is assumed to be 20mm in length, 2 mm in width, and 50 µm deep, with an inlet of 300 micrometers and two outlets of 200 micrometers each. It is assumed that a solution of 5 and 3µm polystyrene particles is supplied through the inlet at different flow rates to experience the acoustic field. For this simulation, the following properties of particles are considered**.**

Table 1. The properties of water and the particles.

Item	Viscosity (cp)	Density (kg/m^3)	Compressibility Pa^{-1} [16]
Water	.89	1000	$5e-10$
Polystyrene 5,3µm		1050	$2.16e-10$

Table 1 outlines the properties of water and polystyrene in terms of their flow resistance, density, and compressibility. In this simulation, polystyrene is denser and less compressible than water. The resonance frequency, according to equation 2, is 375KHZ. The current model is limited to being applied to a single node. However, multiple nodes in the same sample can be observed using this model. The simulation incorporates several runs considering different flow rates (50,100,150µl/hr.) to determine the channel's highest sorting insight.

Result and discussion: The graph in fig:1 illustrates the trajectories of 5 µm and 3 µm particles in a microfluidic channel under acoustic forces over 40 seconds. The red line indicates the 5 μ m, and the blue line represents the 3 μ m particles. The 5 μ m particles are more dominant by the acoustic force since they show much more displacement inside the channel than the other particles. The acoustic pressure applied in this simulation is 0.45 Mpa. It was noted that the more the acoustic pressure is, the more particle displacement is inside the channel. The study found a strong connection between the acoustic field used and how well particles were sorted. When the flow rates are between $100-200\mu l/hr$, particles start separating based on size and density. Smaller and less dense particles move toward the pressure nodes, while the pressure antinodes attract larger and denser particles. The best sorting results are found at moderate flow rates (100 μ l/hr.), where the acoustic radiation force can influence the particles effectively without being hindered by drag forces. Additionally, the acoustic contrast factor is identified as a key factor affecting the direction and extent of particle movement within the fluid. These findings demonstrate the effectiveness of acoustic sorting as a precise and efficient medium for separating particles in microfluidic systems. It is also observed that keeping all other parameters (particles' diameter, channel dimensions, acoustic energy, etc.) constant, the flow rates need to adjust to have the highest efficiency.

Fig. 1: Particles diffusion in the presence of acoustic force.

However, the analysis has some limitations, like particle size and concentration, environmental effect, position of piezo, simplified assumption, and computational limitations. Overall, this simulation results conclude that by tracking the path line of particles, a novel fabricated channel for particle sorting can be established where the particles' mixture will be supplied from the syringe pump through the inlet at specific flow rates and separated into different outlets.

Fig. 2: proposed experimental setup for the particle sorting.

Fig. 2 represents the experimental procedure for the particle sorting mechanism where a channel can be fabricated using soft lithography and PDMS to verify the simulation result. According to the simulation, the 5 µm particles should be collected to the upward outlet, and 3 µm particles should be directed to the middle outlet. The piezo should be attached at the back of the cover glass of the PDMS channel, which will be connected to the amplifier for creating acoustic waves inside the channel.

Conclusion: The current project is focused on the particle's behavior inside a microfluidic channel under acoustic radiation force. Considering the different parameters of eq. 8, the simulation depicts the location of the particles with respect to time. Different parameters are considered to see the impact of acoustic force on the particles. The particles are expected to move toward the pressure node or pressure antinode and discharge through the two outlets. The outcome of this project is expected to motivate the ongoing research work in this field. However, future work would simulate this behavior, considering the acoustic streaming with a more complex design and model. Utilization of machine learning techniques to optimize the acoustic wave parameters for efficient particle sorting needs to be established. Conducting experiments to validate and refine the numerical models based on empirical data is essential before practical implementation.

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