

# Supplementary Information

## High-efficiency inertial separation of microparticles using elevated columned reservoirs and vortex technique for lab-on-a-chip applications

Amir Mohamadsharifi<sup>1</sup>, Hassan Hajghassem<sup>1\*</sup>, Mahsa Kalantar<sup>1</sup>, Ali Karimi<sup>2</sup>, Mirmaghsoud Tabatabaei Asl<sup>1</sup>, Seyedmajid Hosseini<sup>3</sup>, and Majid Badieirostami<sup>4</sup>

<sup>1</sup> Faculty of New Sciences and Technologies, University of Tehran, Tehran, Iran

<sup>2</sup> Department of Chemical and Petroleum Engineering, Sharif University of Technology, Tehran, Iran

<sup>3</sup> Division of Electrical and Computer Engineering, Louisiana State University, Baton Rouge, LA, USA

<sup>4</sup> School of Electrical and Computer Engineering, College of Engineering, University of Tehran, Tehran, Iran

\* Correspondence: hajghassem@ut.ac.ir

**Numerical simulations:** Fluid flow simulations were conducted using COMSOL Multiphysics 6.0 software. The momentum and continuity equations (Eqs. 1 and 2) were solved for a single-phase Newtonian fluid. The fluid's density ( $\rho$ ) and dynamic viscosity ( $\mu$ ) were set to  $1000 \text{ kg/m}^3$  and  $8 \times 10^{-4} \text{ Pa}\cdot\text{s}$ , respectively.  $\vec{u}$  and  $P$  are fluid velocity vector and pressure, respectively. The geometries were meshed using free-tetrahedral elements (Fig. S1A). To ensure mesh independence, a mesh convergence analysis was performed. The z-direction velocity profile of the fluid (Fig. S1B) was plotted along a cut-line illustrated in Fig. S1A by varying the number of mesh elements (from 134,640 to 680,779). The analysis showed that increasing the number of mesh elements did not significantly affect the main profile but only influenced the maximum and minimum values. Therefore, the highest number of mesh elements supported by the computing system, i.e., 680,779, was used to obtain more accurate results.

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho[\vec{u} \cdot \nabla \vec{u}] = -\nabla P + \mu \nabla^2 \vec{u} \quad \text{Eq. 1}$$

$$\nabla \cdot \vec{u} = 0 \quad \text{Eq. 2}$$

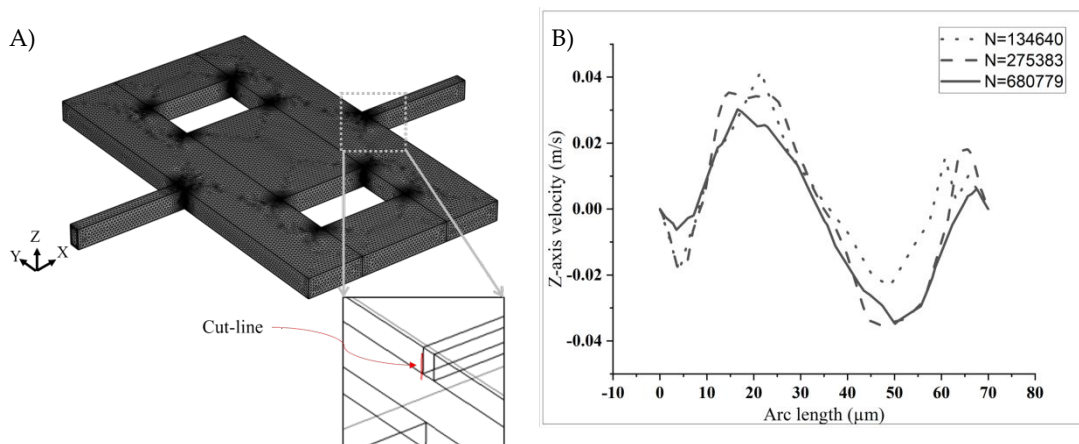


Fig. S1 (A) Schematic representation of the mesh structure utilized for the simulations. The red line indicates the location used for comparing velocity profiles during the mesh independency analysis. (B) Comparison of z-direction velocity profiles along the red line in the microchannel, where vertical flow intensifies, for different numbers of mesh elements (N). Negative velocities indicate downward fluid motion

along the channel height. The solid line corresponds to the final mesh configuration employed for the simulations.

To simulate the particle trapping behavior, we utilized the Lagrangian particle tracing module coupled with the fluid flow simulation. The motion of the particles was determined by solving Newton's second law (Eq. 3). The parameters involved in the equation are the particle mass  $m_p$  and velocity  $u_p$ . In our simulations the particles had a radius ( $a$ ) of  $10\ \mu\text{m}$  and  $4\ \mu\text{m}$ , and a density ( $\rho_p$ ) of  $1050\ \text{kg/m}^3$ .

$$m_p \frac{d\vec{u}_p}{dt} = \sum F_{\text{exerted}} \quad \text{Eq. 3}$$

The exerted forces ( $F_{\text{exerted}}$ ) on the particles during simulations included the viscous drag force ( $F_{\text{drag}}$ ), lift forces (wall-induced lift force  $F_{\text{WIL}}$  and shear-gradient lift force  $F_{\text{SGL}}$ ), pressure gradient force ( $F_{\text{PG}}$ ), and virtual mass force ( $F_{\text{VM}}$ ). The calculation of the viscous drag force was simplified using the Stokes drag formula (Eq. 4) where  $\vec{u}_p$  represents the velocity vector of the particle. The lift force was determined by considering both shear-gradient and wall-induced forces. Eq. 5 and Eq. 6 were utilized to calculate the shear-gradient and wall-induced lift forces, respectively. These equations involve parameters such as  $C_{\text{SGL}}$ ,  $C_{\text{WIL}}$ ,  $U_{\text{max}}$  and  $D_h$  which represent the lift coefficients, maximum fluid velocity, and channel height, respectively<sup>50</sup>. The pressure gradient force ( $F_{\text{PG}}$ ) arises from the pressure difference across the particle's surface, while virtual mass force ( $F_{\text{VM}}$ ) represents the reaction force exerted on a moving particle by the surrounding fluid. The mathematical expressions for ( $F_{\text{PG}}$ ) and ( $F_{\text{VM}}$ ) can be described by Eq. 7 and Eq. 8, respectively.

$$\vec{F}_{\text{drag}} = 6\pi\mu a(\vec{u} - \vec{u}_p) \quad \text{Eq. 4}$$

$$\vec{F}_{\text{SGL}} = C_{\text{SGL}}\rho U_{\text{max}}^2 \frac{a_p^6}{D_h^4} \quad \text{Eq. 5}$$

$$\vec{F}_{\text{WIL}} = C_{\text{WIL}}\rho U_{\text{max}}^2 \frac{a_p^3}{D_h} \quad \text{Eq. 6}$$

$$\vec{F}_{\text{PG}} = \frac{\rho_p}{\rho}(\vec{u}_p \nabla \vec{u}) \quad \text{Eq. 7}$$

$$\vec{F}_{\text{VM}} = \frac{1}{2} \frac{\rho d(\vec{u} - \vec{u}_p)}{\rho_p dt} \quad \text{Eq. 8}$$

During the particle tracing simulation, the wall boundary condition was set to account for particle bouncing off the walls. A time-dependent solver was used, and the simulation was conducted with a time step of  $3 \times 10^{-5}$  second for the constant height and  $4 \times 10^{-5}$  for the elevated chip. The simulation was performed for a duration of 0.1 and 0.4 second in each respective case.

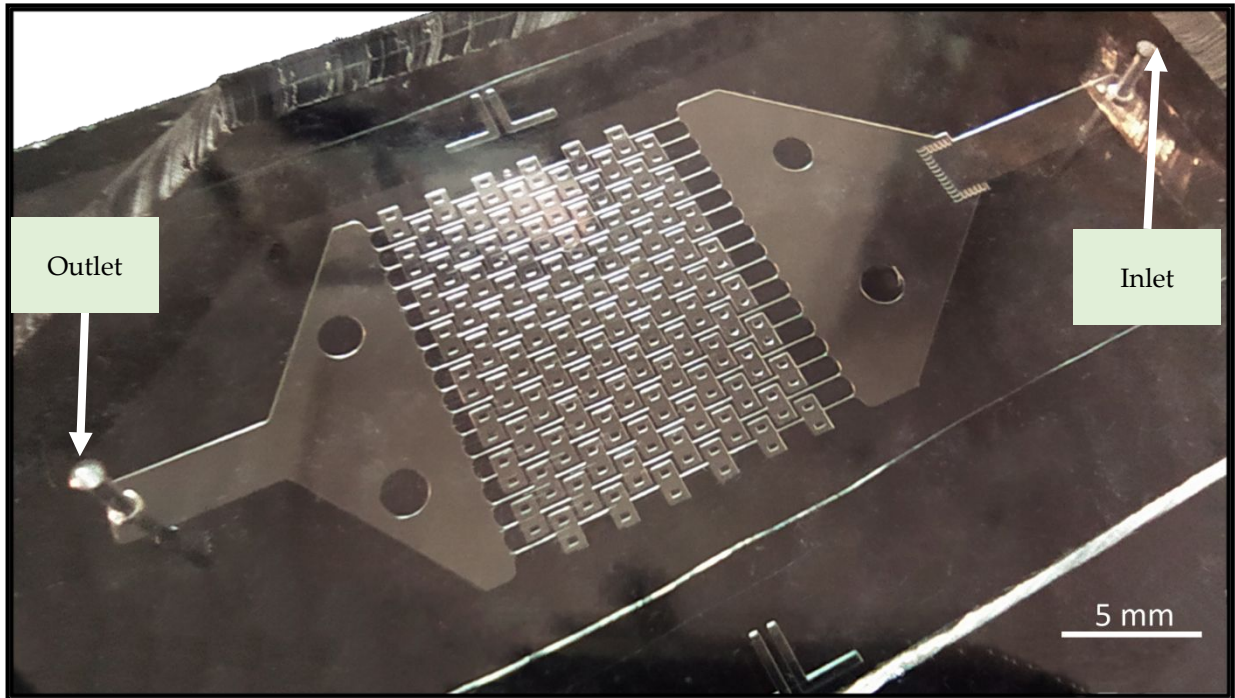


Fig. S2 Fabricated chip containing 16 parallel channels.

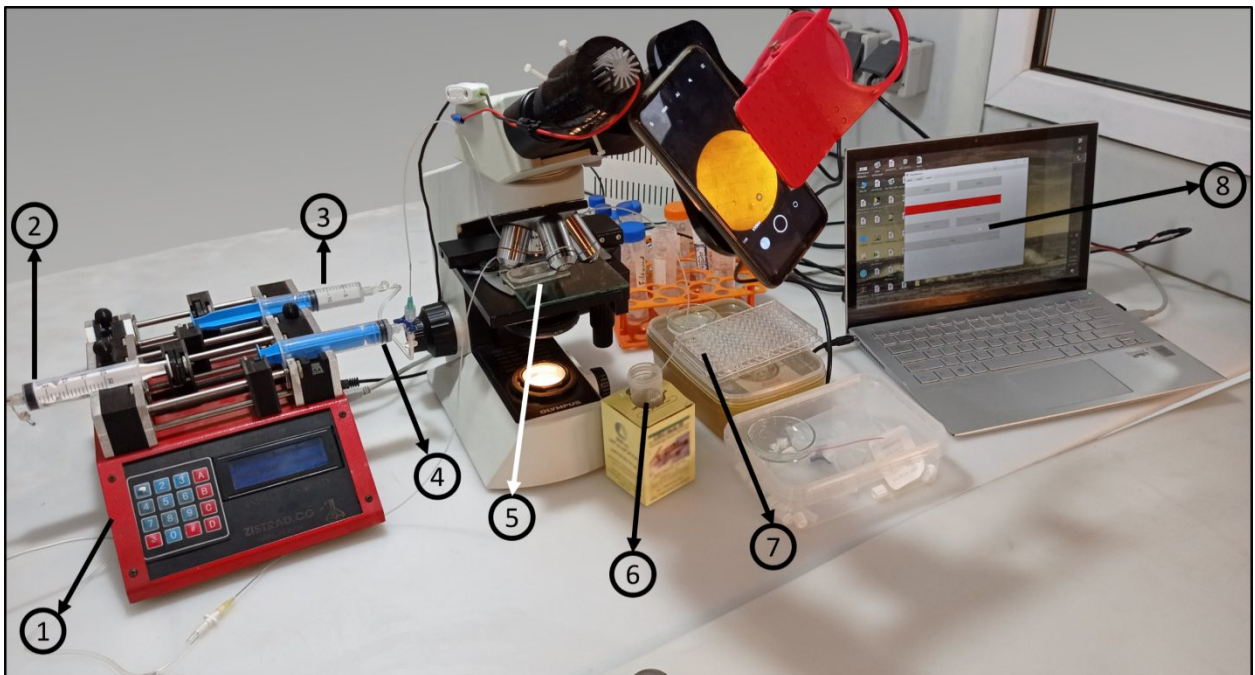


Fig. S3 Test setup including 1- Syringe pump 2- Ethanol syringe (for removing air within the chip) 3- PBS syringe 4- Sample syringe (PBS + microbeads) 5- Chip 6- Waste outlet 7- Main outlet (96 well-plate) 8- Online controlling program by a PC.

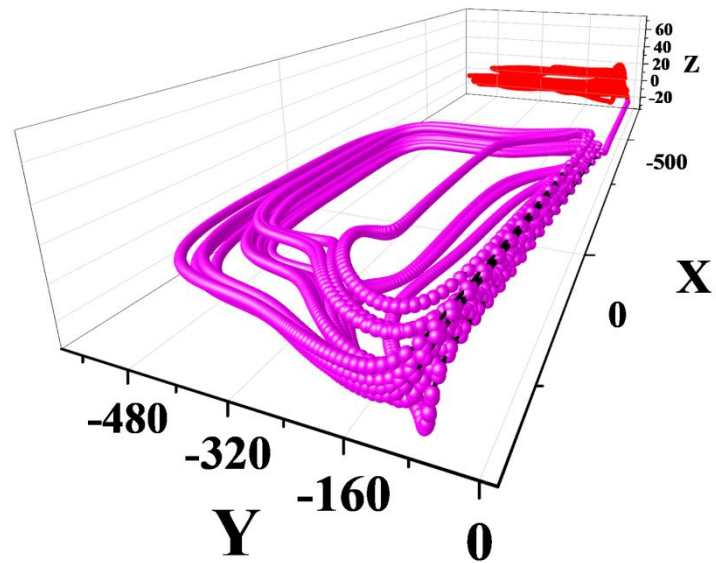


Fig. S4 3D particle trajectory of a 20  $\mu\text{m}$  particle in the ECR chip after 0.4 s into the simulation.

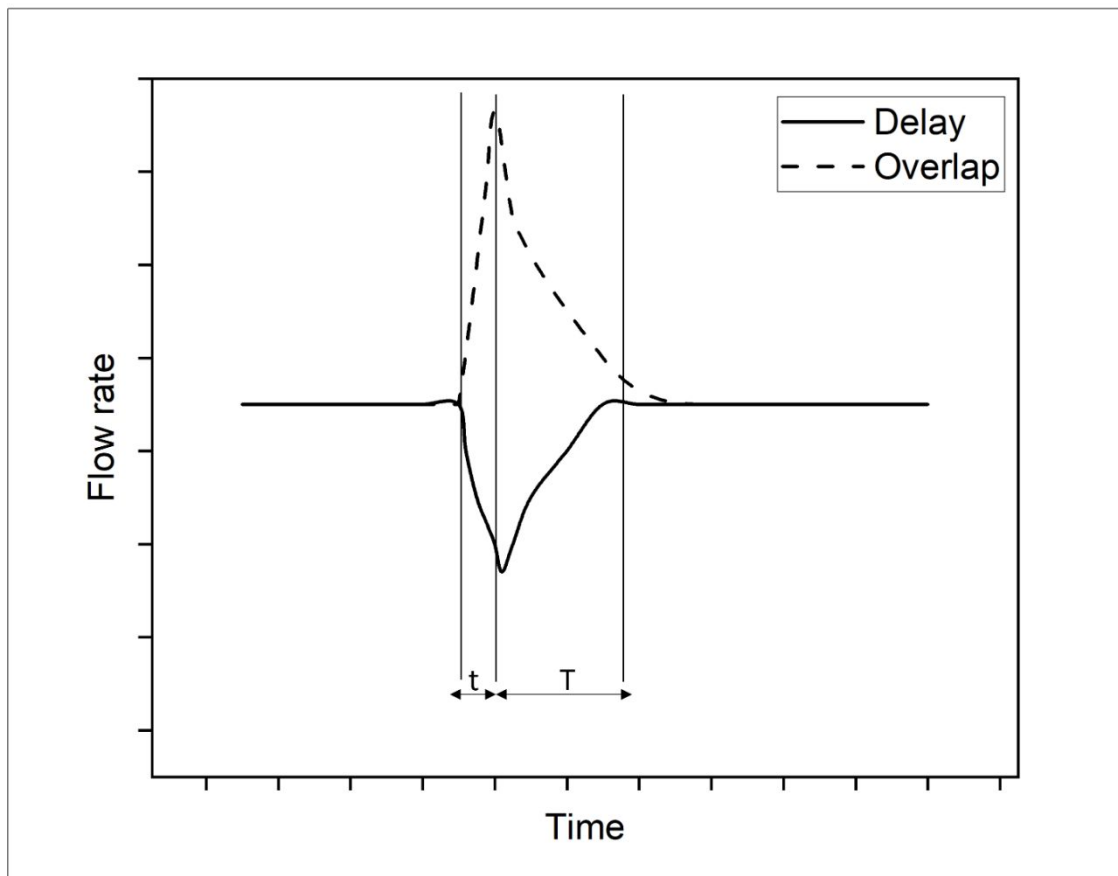


Fig. S5 Schematic representation of the mismatch between injection steps when there is no central controller unit present. The symbol "t" represents the delay time between changing syringes, which leads to a drop-down flow rate or a sudden increase in a short time (less than a second). The symbol "T" represents the adjustment of the flow rate after the injection mismatch, which may take a few seconds. A fully controlled pump resulted in a highly stable flow rate without any significant drop or rise. It is important to change the solution when particles orbit within the reservoirs and the sample is finishing. Changing the flow rate, either increasing or decreasing it, affects the particles' paths and may cause them to exit the reservoir.