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Water Purification in Micromagnetofluidic Devices: Mixing in MHD Micromixers

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Abstract

This contribution addresses a possible solution for water purification from heavy metals by magnetic nanoparticles in microfluidic water flow systems. In this technique, the most important component is the micromixer while efficient mixing and particle driving is achieved by external magnetic fields. For the simulation of water flow and nanoparticles, Computational Fluid Dynamics methods are used. The 2D and 3D Navier-Stokes equations are solved for the flow field while trajectories of the magnetic nanoparticles are simulated by the use of a Lagrangian method. Compared to traditional techniques, this method is expected to succeed chemical speed and increased water purification times.

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Keywords: Water purification; Heavy metals; Micromixers; Microfluidic mixing; Magnetohydrodynamics; Microchannel; Magnetic nanoparticles

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1. Introduction

Reliable methods are needed to detect and remove heavy metals from environmental samples. The basic novelty that is introduced herein is the coupling of nanoparticle science to microfluidics and magnetohydrodynamics for the purification of water [1]. In micro scale devices, due to the absence of turbulence (low Reynolds number), the mixing is a slow procedure. To resolve this problem a magnetohydrodynamic (MHD) micromixer is the innovating application which demonstrates the basic principle that instead of large stirring water tanks that may be used for the nanoparticles to uptake slowly the heavy metals, a micromagnetofluidic structure [2] accelerates the chemical reaction rates.

Micromixers have attracted considerable interest because they enhance micromixing. They can be classified into active and passive ones [3]. Passive mixers do not require external actuation to improve mixing, they achieve mixing because of their microchannel configurations, they have no moving parts and they do not consume energy. The mixing process relies on molecular diffusion or chaotic advection and causes homogeneous mixing. Active mixers use external disturbance to enhance the mixing process. They are categorized according to the types of disturbance, as: Electrohydrodynamic, Pressure driven, Dielectrophoretic, Electrokinetic, Magnetohydrodynamic, Acoustic, Thermal, etc. Convection is the main mixing mechanism in active micromixers and creates heterogeneous mixing [4].

The innovation that is presented herein provides a microfluidic device in order to bring magnetic nanoparticles (MNPs) and heavy metals close enough to chemically react faster when MNPs are transported in water microchannels. If particles and heavy metals are nearby, hydrodynamic interactions build up between them, giving rise to some dynamics. This system is a well-known micromagnetofluidic structure that exerts both attractive and repulsive forces at the micrometer scale. When a particle moves in a microchannel, it is slowed down by the walls and consequently generates horizontal eddies. The MHD micromixers can produce excellent micromixing in the flow due to the utility of external magnetic forces. The factors that determine the actuation forces on the magnetic particles and affect the micromixing are: the applied current, the geometry of the electromagnet, the magnetization moments of the magnetic particles, the size of the magnetic particles, the relative position of the microchannel to the electromagnet [5].

The research effort is focused here on MHD micromixer which is sketched in Figure 1. To actuate magnetic particles, a macro-sized external permanent electromagnet was used [6]. The magnetic forces actuated the magnetic particles to move in the microchannel and by switching the electromagnets on and off alternatively, the micromixer could generate periodic magnetic forces that agitated the magnetic particles to oscillate along the desired direction of the microchannel. The mixing efficiency was improved due to the interaction of the fluids and magnetic particles.

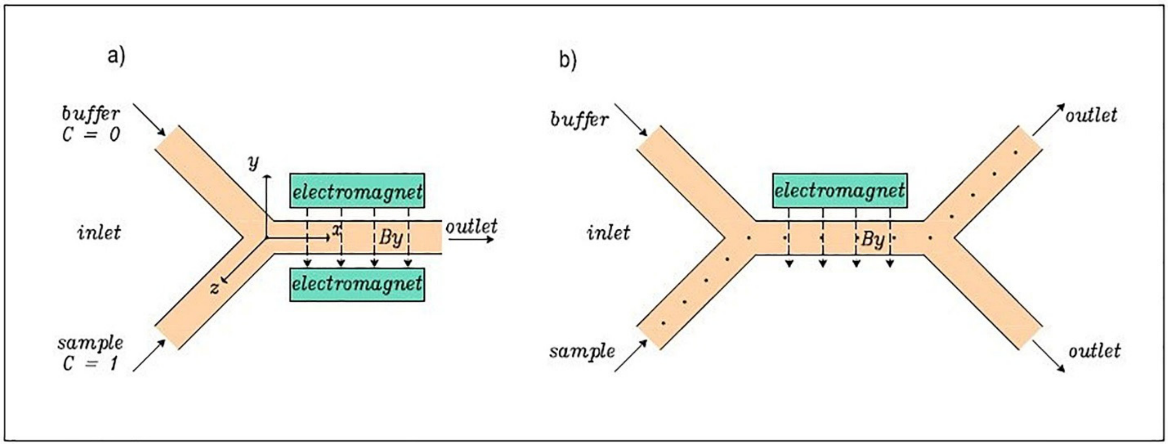

Fig. 1. (a) Schematic diagram of the magnetic micromixer's geometry, for the present computational method; (b) The magnetic particles' motion under the magnetic field of the external magnets.

This paper presents a computational method for water and spherical magnetic particles flow. The simulation method is used to find the optimal values of gradient magnetic field which will guide the largest percentage of particles in the microchannel and will achieve the maximum mixing efficiency. The results of simulations are compared with analytical ones (see Figures 3,4) . The theory and the forces that have been incorporated into the numerical model are presented in Section 2. The computational results and the comparison to the analytical results take place in Section 3. Finally, the conclusions from this research are presented in Section 4.

2. Methodology

In this research paper, the computational area is the mixing microchannel. The shape - dimensions of the channel and the positions – concentration of the particles are shown in Figure 2. This model contains all the forces which act on particles, some forces can be neglected in MHD micromixer studies [6,7] as it is shown in part 2.1.

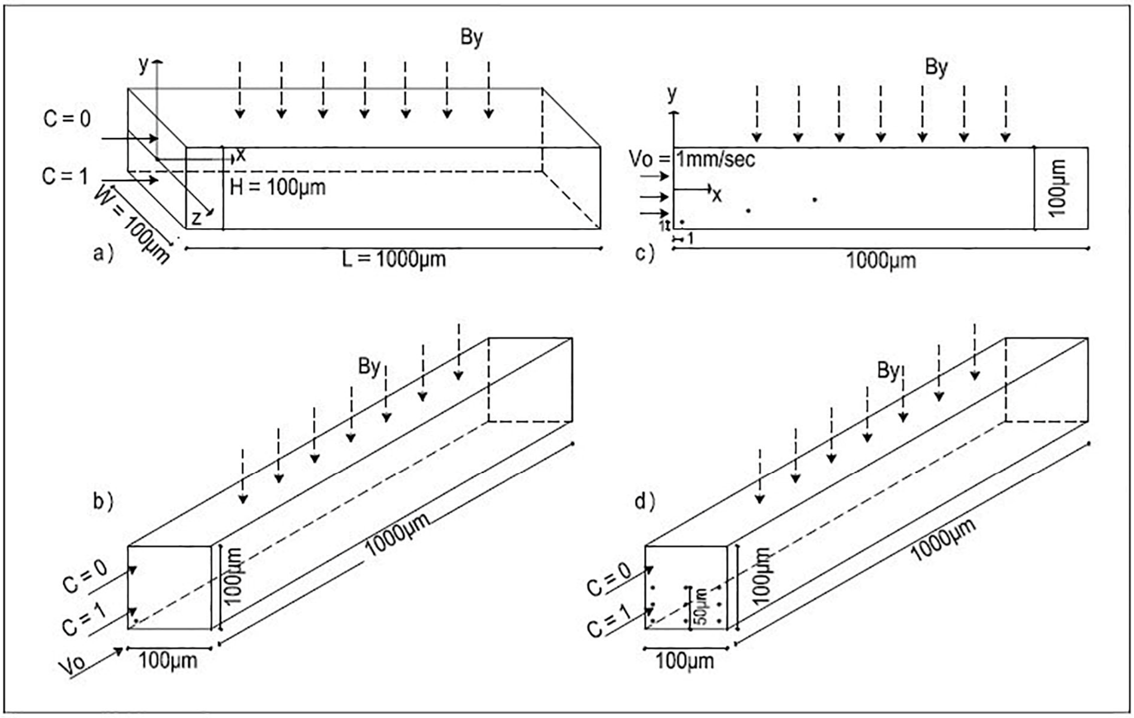

Fig. 2. Schematic diagram of the (a) Mixing microchannel; (b) One particle's position at the bottom half of channels entrance; (c) Particle's trajectory; (d) Nine particle's position at the bottom half of channels entrance.

2.1. Mathematical model

The equations that are involved in this model are described below.

For the fluid motion:

The incompressible fluid flow is expressed by the continuity and Navier-Stokes equations:

$$\nabla \cdot \vec{V} = 0 \tag{1}$$

$$\rho_f\left(\frac{\partial \vec{V}}{\partial t} + (\vec{V} \cdot \nabla)\vec{V}\right) = -\nabla P + \eta \nabla^2 \vec{V} + \vec{F_d} \tag{2}$$

where $\vec{F_d}$ is the drag force exerted by a magnetic particle on the fluid element, $\vec{V}$ is the velocity vector of fluids, ρ_f is the density of fluid, P is the pressure and η is the dynamic viscosity of the fluid.

The simplified mass transport equation in an incompressible flow is described as:

$$\frac{\partial C}{\partial t} + \vec{V} \cdot \nabla C = D\nabla^2 C \qquad (3)$$

where C is the dimensionless concentration, D is the diffusion coefficient which is constant.
For the MNPs motion:
The motion of the magnetic particles is governed by the Newton's second law:

$$m_p \frac{d\vec{v}}{dt} = \vec{F_d} + m_p\vec{g} + \vec{F_m} \qquad (4)$$

where $m_p\vec{g}$ is the gravity force of each magnetic particle equal to 8.1×10-3 pN and can be neglected in comparison to the large magnetic actuation force, F_d is the drag force and can be calculated from the Equation 5,

$$\vec{F_d} = C_D\rho_f(\vec{V} - \vec{v})|\vec{V} - \vec{v}|\frac{A_p}{2} \qquad (5)$$

where C_D is the drag coefficient and depends on the Reynolds number, $\vec{V}$ and $\vec{v}$, is the velocity vector of fluid flow and of the magnetic particles respectively, A_p is the cross-section area of the particles and ρ_f is the fluids density. The magnetic force exerted on the magnetic particles can be calculated by Equation 6,

$$\vec{F_m} = V_p(\vec{M} \cdot \nabla)\vec{B} \qquad (6)$$

where $\vec{F_m}$ is the magnetic force, V_p is the particle volume, $\vec{M}$ is the magnetization of the particle and $\vec{B}$ is the flux density generated by the external electromagnets [8]. Due to the electromagnets, the magnetic field in y direction is stronger than that in x, z direction. So, the components B_x , B_z can be neglected and the corresponding magnetic actuation force F_m is significant only along the y direction. As a result, the Equation 2 can be simplified as:

$$F_{my} = V_p M_s \frac{\partial B_y}{\partial y} \qquad (7)$$

2.2. Boundary and initial conditions

Boundary conditions are set as the fluid flow enters the microchannel at an inlet constant velocity V_0=1mm/s. The initial velocities of MNPs are the same as that of the fluids. The stream of buffer with concentration C=1 enters from the bottom half of the channel and the stream of sample with C=0 enters from the upper half of the channel (see Figure 2a). MNPs enter the microchannel in two different ways. Firstly, one particle enter the microchannel from the lower left corner of the bottom half of the channel with a velocity equals to the local velocity of the fluid. Secondly, nine particles enter the microchannel from nine determined locations of the bottom half of the microchannel entrance (see Figure 2d). No-slip boundary condition is applied on the microchannel's walls. At the outlet, constant pressure condition is applied. The fluid flow field and concentration (see Figure 2d) are set as the initial conditions for our simulation.

2.3. Numerical model

We assume that the properties of the carrier electrolyte fluid are the same as that of water (see Table 1). The numerical model is set in a first place with a single particle and in a second phase with nine particles. The dimensions of the 2D microchannel are: L=1000μm and W=100μm [9].

Table 1. MNPs and Fluid Properties

Property of MNPs			Property of Fluid		
Susceptibility of the particle	Xp	11.3	Permeability of free space	μ0	4π*10-17 N/A2
Particle radius	rp	0.5*10-6 m	Relative permeability of the fluid	μr	1.0
Particle volume	Vp	5.236*10-19 m3	Carrier fluid density	ρf	1000 Kg/m3
Particle density	ρp	1580 Kg/m3	Carrier fluid density viscosity	η	1*10-3 Kg/ms
Particle mass	mp	8.27*10-16 Kg			

For the analytical solution, we calculated By, where y in meters,

$$B_y = \sqrt{2(y + 50 \cdot 10^{-6})} \tag{8}$$

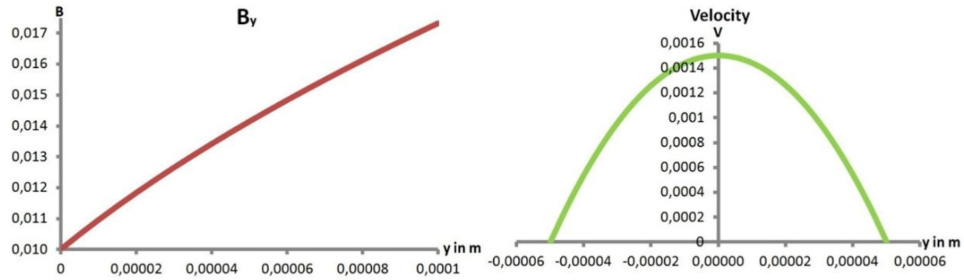

Fig. 3. Schematic diagram of the magnetic field By and the fluid's velocity Vx

and the fluid velocity (see Figure 5) where, V0= 1 mm/s,

$$V_x(y) = \frac{3}{2}V_0(1 - \frac{4y^2}{W^2}) \tag{9}$$

The magnetic and hydrodynamic drag force on particles are calculated respectively from:

$$F_{my} = V_p M_s \frac{\partial B_y}{\partial y} = \frac{V_p \chi_p B_y \frac{\partial B_y}{\partial y}}{\mu_0 \mu_r} \tag{10}$$

$$\mathbf{F_{dx} = -6\pi\eta r_p(v_x - V_x)} \tag{11}$$

$$\mathrm{F_{dy} = -6\pi\eta r_p(v_y - 0)} \tag{12}$$

Solving the governing equations (13) and (14) of particles:

$$m_p \frac{dv_x}{dt} = F_{dx} = -6\pi\eta r_p(v_x - V_x) \tag{13}$$

$$m_p \frac{dv_y}{dt} = F_{dy} + F_{my} = -6\pi\eta r_p v_y + \frac{V_p \chi_p B_y \frac{\partial B_y}{\partial y}}{\mu_0 \mu_r} \tag{14}$$

We obtained the particles velocity,

$$\boldsymbol{v_x} = \boldsymbol{v_{x0}} e^{-c_1 t} + \boldsymbol{V_x}(\mathbf{1} - e^{-c_1 t}) \tag{15}$$

$$\boldsymbol{v_y} = \boldsymbol{v_{y0}} e^{-c_1 t} + \frac{c_2}{c_1}(\mathbf{1} - e^{-c_1 t}) \tag{16}$$

where $c_1 = \frac{6\pi\eta r_p}{m_p}$ and $c_2 = \frac{\frac{V_p \chi_p B_y \frac{\partial B_y}{\partial y}}{\mu_0 \mu_r}}{m_p}$

Finally, the particle's trajectory (see Figure 4) was calculated:

$$\boldsymbol{x} = -\frac{\boldsymbol{2V_0}}{\boldsymbol{W^2}} \frac{\boldsymbol{c_1}}{\boldsymbol{c_2}} [\boldsymbol{y_p}(\boldsymbol{y_p^2} - \frac{\mathbf{3}}{\mathbf{4}}\boldsymbol{W^2}) - \frac{\boldsymbol{W^3}}{\mathbf{4}}] \tag{17}$$

2.4. Numerical method

For the simulation of the water flow and nanoparticles motion inside the magnetic microchannel we use Computational Fluid Dynamics methods based on the open source library OpenFOAM. For the flow field, the Navier-Stokes equations are solved while the particles' trajectories are simulated by the use of Lagrangian method. The implicit Euler method is used for solving equations. The time step for all numerical results is 10^{-6} s. To solve the motion of fluid and particles in the microchannel, we firstly solve the flow equations and then the MNPs equations. The influence of the magnetic field was imposed then to the model. This method is based on an algorithm that focuses on particles desired trajectory (see Figure 4) to be away from microchannel's walls due to the desired optimum gradient magnetic field and will achieve the maximum mixing efficiency in the mixing microchannel.

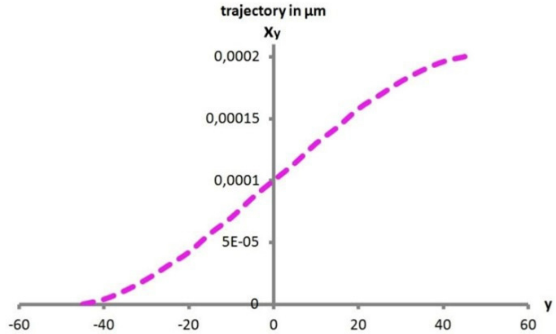

Fig. 4. Schematic diagram of the particle's trajectory (see in Figures 2c, 2d the cross section of the microchannel).

3. Results

The geometry for this computational method appears in Figure 1. In this paper, the model is limited only in the straight part of the two dimensional channel, as it is shown in Figures 2 and 5. The lengthwise dimension of the microchannel is 1000μm, the widthwise dimension is 100μm and the height is 100μm. The results were obtained by using a mesh of 3552 quadriteral cells. The fluid was water and the magnetic particles' diameter was 1μm.

Two different simulations were carried out in order to calculate all the model's parameters. In the first case, a single spherical particle was injected, as it is shown in Figure 2b, and there was almost any influence to the fluid's motion due to its presence in the channel. In the second case nine spherical particles were injected, as it is shown in Figure 2d in the mixing microchannel. The results of their influence in the flow field are depicted in section 3.1.

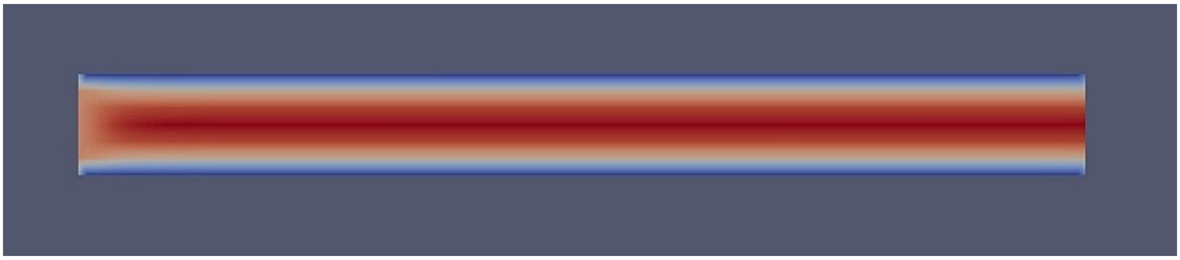

Fig. 5. Fluid velocity in the microchannel.

3.1. Flow field and effect of magnetic field

Figure 1 shows the magnetic micromixer which consists of a pair of external electromagnets. A constant and homogeneous magnetic field is applied to the present simulation. The magnetic forces that are created from the application of current to one electromagnet, actuate the magnetic particles to move in the microchannel and by switching the electromagnets on and off alternatively, the micromixer can generate periodic magnetic forces that agitate the magnetic particles to oscillate along the desired direction of the microchannel. Figures 6 and 7 show the applied magnetic field Hy which is in the range of (8.5951e+03, 1.339e+03) A/m . The shades of red lines depict stronger magnetic field as the blue ones refer to a weaker magnetic field.

Fig. 6. MNPs movement: applied magnetic field when the magnet is switched on.

In Figures 6 and 7, we can observe the position of the nine MNPs. Due the periodic magnetic forces they follow the desired trajectory away from the channel walls.

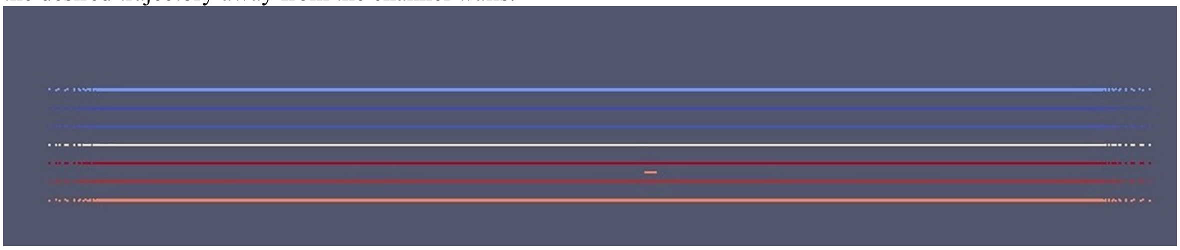

Fig. 7. MNPs movement: applied magnetic field when the magnet is switched off.

Magnetic nanoparticle's oscillating motion is shown in Figure 8. If the magnetic field is weak enough, the MNPs move to one direction and stay on the wall until the magnetic forces are reversed. On the other hand, if the magnetic field is strong enough, then the magnetic particles only oscillate and do not enhance the micromixing. The optimum gradient magnetic field drive the MNPs away from the channel walls and create a better mixing efficiency.

Fig. 8. MNPs oscillating movement along the y-direction due to the applied magnetic field.

We have better mixing results with the oscillating MNPs movement, due to the presence of periodic magnetic forces and switching frequency.

4. Conclusions

This research paper presented a computational method for the simulation of magnetic particles coated with appropriate metal oxides to capture heavy metals from water solution in microchannels. Due to lack of turbulence, a magnetically driven micromixer configuration is considered to enhance mixing. In the present numerical work, in order to simulate the mixing process, we firstly solve the flow equations and then the discrete MNPs equations with the influence of the magnetic field to act only in particles. The improvement of particles velocity and trajectory under various external magnetic fields and the mixing efficiency in a fluid environment is the purpose of the present work. The optimum gradient magnetic field helped the navigation of particles into a desired trajectory away from the channel walls. As a result, a better and faster mixing between particles and fluid took place. Comparison of computational and analytical results showed in the second and third part of this work is found to be in accordance to the results of [9]. Since we are confident on its performance, the model will be used to further improve the heavy metal capture method.

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