Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 162 (2016) 77 – 82

Procedia Engineering

www.elsevier.com/locate/procedia

International Conference on Efficient & Sustainable Water Systems Management toward Worth Living Development, 2nd EWaS 2016

# Computational study of the optimum gradient magnetic field for the navigation of the spherical particles in the process of cleaning the water from heavy metals

Evangelos G. Karvelas[a,]*, Nikolaos K. Lampropoulos[b], Theodore E. Karakasidis[a], Ioannis E. Sarris[b]

[a]*Department of Civil Engineering, University of Thessaly, Volos, 38334 ,Greece*
[b]*Department of Energy Technology, Technological & Educational Institute of Athens, 12210, Greece*

---

## Abstract

The usage of magnetic spherical nanoparticles, coated with substances and driven to targeted areas in tanks, is proposed for cleaning the water from heavy metals. In the present paper, a computational study for the estimation of the optimum gradient magnetic field is presented in order to ensure the optimum driving of the particles into the targeted area. The optimization of the gradient magnetic field rates' is verified with the particles' deviation from a desired trajectory. Using the above mentioned method, it was depicted that with the increase of the optimization parameters number, the particles' deviation from the desired trajectory is decreased.

*Keywords:* Magnetic driving; Nanoparticles; CFD; Waste water; Heavy metals

---

## 1. Introduction

Increasing pollution of groundwater and surface water from a wide variety of industrial, municipal, and agricultural

---

* Corresponding author. Tel.: +30-210-538-5382; fax: +30-210-538-5306 .
*E-mail address:* karvelas@civ.uth.gr

doi:10.1016/j.proeng.2016.11.017

sources has provoked serious water quality problems in these water resources, resulting in a reduction of the supply of freshwater for human use [1]. Although the nature of pollution problems may vary, they are typically due to inadequate sanitation, algal blooms, detergents, fertilizers, pesticides, chemicals, potentially toxic metals, salinity caused by widespread and inefficient irrigation, and high sediment loads resulting from upstream soil erosion [2]. Thus, water scarcity is being recognized as a present and future threat to human activity and as a consequence, water purification technologies are gaining major worldwide attention [3]. In this perspective, biochemical or biotechnological nanotechnology has been identified as one of the most promising technologies that could play an important role in resolving many of the problems involving water purification and quality [4].

Treatment and remediation of water contaminated with hazardous substances may be one of the most significant environmental applications of nanotechnology, led by nanoparticles. Among the nanosized materials, iron oxides play a major role in many areas of chemistry, physics, and materials science. In particular, magnetic iron oxides such as magnetite (Fe3O4) and magnetite (ϒ-Fe3O4) have been investigated intensively for environmental applications [5]. Facilitated separation from water by magnetic force is the most attractive property of magnetic nanoparticles. In addition to convenient magnetic properties and low toxicity and price, iron oxide (e.g., Fe3O4) nanoparticles present many advantages, as for instance: 1) magnetic properties, 2) low toxicity and price, and 3) high surface to volume ratio (depending on the particle size), which associated to their ability for surface chemical modification can show enhanced capacity for metals uptake in water treatment procedures. Surface modification achieved by attachment of inorganic shells or/and organic molecules not only stabilizes the nanoparticles, eventually preventing their oxidation, but also provides specific functionalities that can be selective for ion uptake. Using paramagnetic nanoparticles the magnetic response of the nanoparticles is maximized since they form chains under the influence of a steady magnetic field. The size of aggregates is very important and it depends on various different parameters [6].

In this study, a computational platform is presented in order to ensure the appropriate rates of the gradient magnetic field. In this way, the optimum driving of nanoparticles to targeted areas and the optimum separation of magnetic nanoparticles from clean water is achieved. In section 2, the method for calculation the optimum rates of magnetic field is presented. In section 3, the results of the computational platform under the influence of different geometries and different velocities of the fluid are presented. Finally, in section 4, the results and the potential of the present platform are described.

## 2. Methodology

### 2.1. Numerical model

For the driving model of the particles six major forces are considered and described below; the magnetic force from the Main Magnet static field as well as the Magnetic field gradient force from the special Propulsion Gradient Coils. The static field aggregates the nanoparticles, while the magnetic gradient navigates the agglomerates. Moreover, the contact forces among the aggregated nanoparticles and the wall, and the Stokes drag force for each particle are considered, while only spherical particles are used here. In addition, gravitational forces due to gravity and the force due to buoyancy are added. The numerical model for the pre-mentioned forces is given [7]. Finally, attractive forces such as Van der Walls are included in this model.

### 2.2. Numerical method

The OpenFoam platform was used for the calculation of the flow field and the uncoupled equations of particles motion. The simulation process reads as follow; initially, the fluid flow is found using the incompressible Navier-Stokes equations and the pressure correction method. Upon finding the flow field (pressure and velocity), see Figure 1a. The motion of particles is evaluated by the Lagrangian method. The equations are solved in time by the Euler time marching method. The stability of the algorithm is guaranteed through a time step of the order of $10^{-6}$ s. The method is based on an iteration algorithm that intents to minimize the deviation of the particles from a desired trajectory. The trajectory is predefined in the computational platform by a 10th degree polynomial. In this way, the gradient magnetic field is temporarily adjusted in a suitable way such that the particles' distance from the trajectory to be decreased, see Figure 1b. Each alteration of the gradient magnetic field, which is achieved through the computational study, is called an optimization parameter. To verify the optimal gradient magnetic field a Convariance Matrix Adaptation Evolution Strategy (CMAES) was used in order to navigate the particles into the desired area [8], see Table 1.

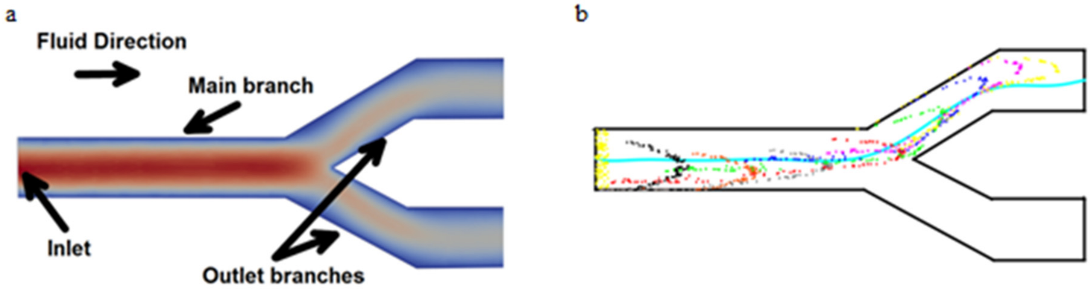

Fig. 1. (a) Y shaped geometry; (b) Desired trajectory (cyan line) and positions of each particle in each time step.

Table1. Values used by the computational platform in order to navigate the particles into the desired trajectory .

| Time step (s) | Color | mT/m |
|---|---|---|
| Initial | Yellow | 0 |
| 0.2 | Black | -499.9 |
| 0.4 | Orange | -500 |
| 0.6 | Grey | 152.9 |
| 0.8 | Red | 482.9 |
| 1 | Green | 500 |
| 1.2 | Blue | 423.9 |
| 1.4 | Pink | 315 |
| 1.6 | Yellow | 9.8 |

## 3. Results

For the evaluation of the potential of this computational method, a series of simulations with different numbers of optimization parameters for the magnetic field and different velocities of the fluid were performed.

For this reason, a (2D) Y-shaped geometry was simulated, as is showed in Figure 1a. The inlet of the fluid is in the left of the geometry and there are two outlet branches in the right side. The angle between the two outlet branches is 60° degrees. The diameter of both the main and outlet branches is 2.5 mm. The overall length of the simulated geometry was 0.036 m and the computational grid was composed by 5012 prism cells. The fluid that was simulated was water under 20°C and the particles' diameter was 11um.

Two series of simulations were performed in order to evaluate the potential of the method under different velocities of the fluid (calculating the particles' distance from the desired trajectory). In the first case, the velocity of the fluid was 12.2 mm/s and 6.1 mm/, while in the second case the velocity was 9mm/s and 4.5 mm/s in the in the main branch and outlet branches of the geometry, respectively. For each series of simulations, 18 optimization parameters were used. The influence of the number of particles into the driving process was also ensured from the computational platform.

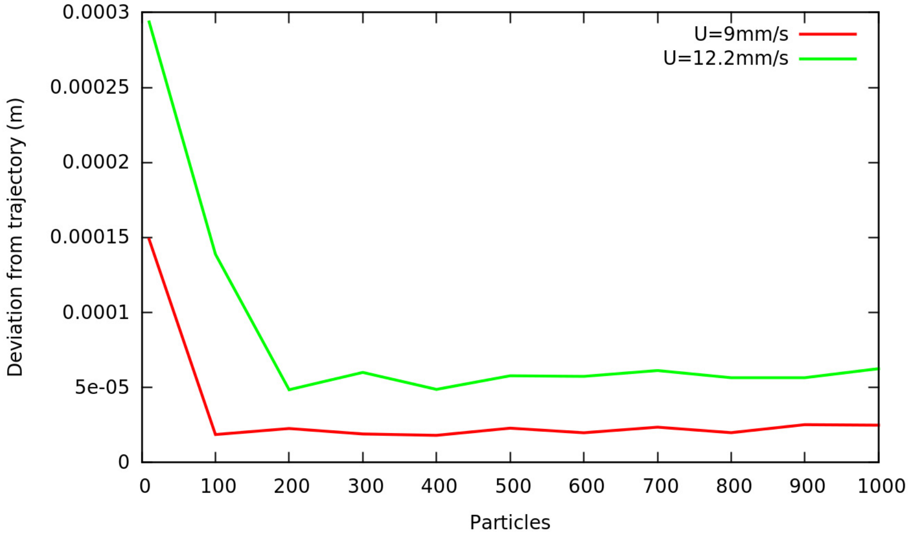

Fig. 2. Deviation of particles from the desired trajectory under two different velocities of the fluid for different number of particles.

In Figure 2, the particles' deviation from the desired trajectory for two different fluid velocities is depicted. The particles' deviation from the desired trajectory was estimated before the particles' issue from the geometry. The velocity of the fluid plays an important role in the driving process. Through the simulations, it is cleared that the higher the velocity is, the bigger the deviation from the desired trajectory is. As a result, the nanoparticles' driving becomes more efficient in tubes with small velocities. To minimize the particles' deviation from the trajectory, the use of higher rates of the magnetic fields is necessary. Alternatively, more optimization parameters can be used.

The computational platform was also used in order to define the geometry's influence during the nanoparticles' driving into the targeted areas. For this purpose, simulations in the geometry of Figure 3 were performed and the results were compared to those from geometry of Figure 1a.

Fig. 3. Y shaped geometry. The inlet of the fluid is in the left of the geometry and there are two outlet branches in the right side. The angle between the two outlet branches is 60° degrees. The diameter of the main and outlet branches are 2.5mm and 1.125mm, respectively. The overall length of the simulated geometry was 0.06 m and the computational grid was composed by 5644 prism cells.

In Figure 4, the nanoparticles' deviation in relation to the tube's height under the influence of 18 optimization parameters and fluid's velocity in the main branch 12.2 mm/s, is depicted. The green line shows the particles' deviation when the tube's elevation is 2.5 mm. The red line depicts the particles' deviation when the tube's elevation is 1.125 mm. Smaller diameters of the tubes lead to smaller deviation of the particles from the desired trajectory and as a result the computational method becomes more efficient.

The importance of the optimization parameters' number is depicted in Figure 5. Simulations were performed in the geometry of Figure 1a with fluid velocity 12.2 mm/s in the main branch. The increase of the optimization parameters number lead to the increase of the number of particles that move on the desired trajectory. In addition, this increase makes the other particles move closer to the trajectory.

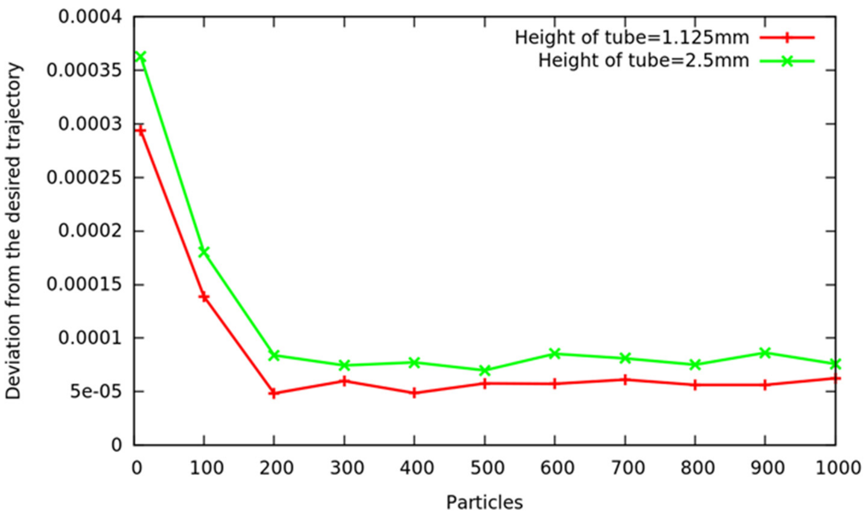

Fig. 4. Deviation of particles from the desired trajectory for two geometries with different height of tube.

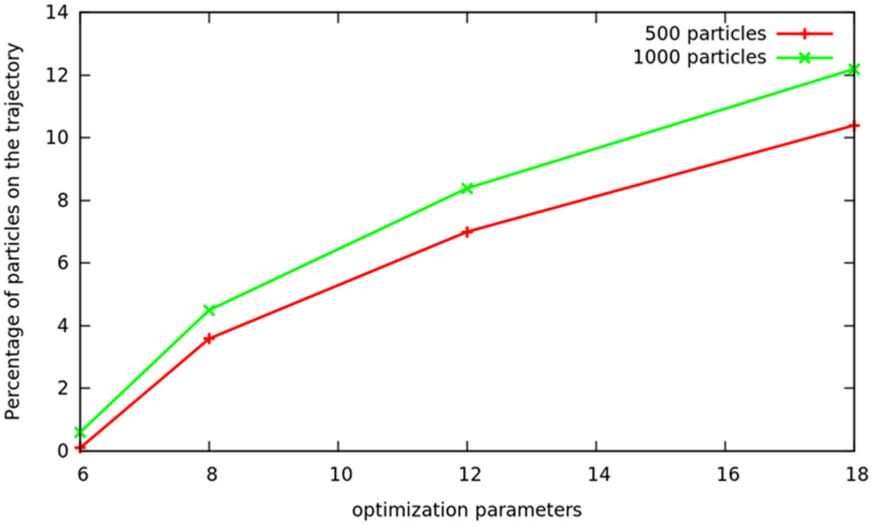

Fig. 5. Percentage of particles on the trajectory under different optimization parameters.

## 4. Conclusions

In this work, a computational study of the optimum gradient magnetic field for the driving of spherical particles into targeted areas is presented. The computational method presented can achieve driving magnetic particles into the desired trajectory with an efficiency above 90%. The results conclude that the more optimization parameters used, the less the particle's distance from the desired trajectory is. The computational platform can be used with optimum efficiency in small tubes and with low fluid velocities. The computational platform has the potential to estimate the appropriate deviation of the magnetic field during the particles' navigation into micromixers. As a result, a better mixing of the particles with the fluid and particles' removal from the microtubes, in order to be re-used, is achieved.

## References

[1] J.A. Foley, R. DeFries, G.P. Anser, C. Barford, G. Bonan, S.R Carpenter, F.S. Chapin, M.T. Coe, G.C. Daily, H.K. Gibbs, J.H. Helkowski, T. Holloway, E.A. Howard, C.J. Kucharik, C. Monfreda, J. Patz, I. Prentice, N. Ramankutty, P.K. Snyder, Global Consequences of Land Use, Science 309 (2005) 570-574.

[2] I.R. Falconer, A.R Humpage, Health risk assessment of cyanobacterial (blue-green algal) toxins in drinking water, J. Environ. Res. Public Health 2 (2005) 43-50.

[3] J. Theron, J.A. Walker, T.E. Cloete, Nanotechnology and water treatment: applications and emerging opportunities, Crit. Rev. Microbiol. 34 (2008) 43-69.

[4] J.Y. Bottero, J. Rose, M.R. Wiesner, Nanotechnologies: tools for sustainability in a new wave of water treatment processes, Integr. Environ. Assess. Manag. 2 (2006) 391-395.

[5] F.B. Li, X.Z. Li, C.S. Liu, T.X Liu, Effect of alumina on photocatalytic activity of iron oxides for bisphenol ; A degradation, J. Hazard Materials 149 (2007) 199-207.

[6] N.K. Lampropoulos, E.G. Karvelas, I.E. Sarris, Computational study of particles interaction distance under the influence of steady magnetic field, Advances in Systems Science and Applications 15 (2015) 227-236.

[7] N.K. Lampropoulos, E.G. Karvelas, I.E. Sarris, Computational modeling of an MRI guided drug delivery system based on magnetic nanoparticle aggregations for the navigation of paramagnetic nanocapsules, 11th World Congress on Computational Mechanics (WCCMXI) Barcelona, Spain 2014.

[8] N. Hansen, The CMA evolution strategy ; a comparing review, Advances on estimation of distribution algorithms 192 (2006) 1769-1776.