Simulations on capture efficiency of magnetic particles transported in a fluidic channel

Prakash Chandra¹, Shashi Sharma² and Anurag Gaur¹, *

¹Department of Physics, National Institute of Technology, Kurukshetra-136119, INDIA
²Department of Mathematics, Indian Institute of Technology, Roorkee-247667, INDIA

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INTRODUCTION

The basic idea of magnetic drug targeting (MDT) is that magnetic particles are used as controllable carriers of medical agents that are attached to the particles. This method of targeting is a promising approach for tumor treatment due to its high targeting efficiency [1, 2]. The main advantage of using magnetizable particles is that the treatment is localized, because the drugs are bound to the nanoparticles which are injected into the blood stream close to the tumor. This reduces overall side effects, compared with chemotherapy, which is a systemic treatment that delivers chemicals to parts of the body, which do not require them. A second advantage is that by adjusting the applied magnetic field, a high concentration of the particles can be attracted to a specific target site and kept there [3]. Recent studies show that an externally applied magnetic field can trap drug loaded polymer coated magnetic carrier nanoparticles (MCNPs) at targeted locations [5–9]. In this method, a suspension of MCNPs is injected into a blood vessel near the tumor [10]. An external magnetic field is applied to localize the MCNPs at the targeted region, maximizing drug concentration at the targeted region and minimizing systemic toxicity and wastage of drugs [6]. The capture of MCNPs loaded with anticancer drug has been primarily investigated for surface tumors [4, 6] and in animal models [11, 6, and 12]. Related magnetic hyperthermia, [13] and radiation therapies [14] have also been studied.

The effectiveness of this technique is critically dependent on MCNPs with superior properties [15]. The flow behaviour of such MCNPs in the blood stream is the key to effective magnetic drug targeting [16]. Micron sized magnetic particles have been deposited in a capillary bed of a blood vessel inside a tumor by placing an external magnetic field by 10 cm away from the tumor location [17]. Parametric analyses of the transport and deposition of magnetic carriers in the microvasculature have been reported by Furlani et al. [18]. The flow rate of the blood, the magnetic and hydrodynamic properties of the MCNPs is very important parameters, which can significantly influence MCNP deposition at the targeted region.

The ideal targeted drug delivery system is the one that delivers the maximum amount of drug to target site. The reality, however, is far away from that ideal scenario. The amount of drug delivered to tumor targets is much less than 5 % at most, which is reported earlier [19]. Our efforts instead may have to be focused on how to better exploit this moderate amount of the drug delivered to the target tumor. Therefore, in this study, we try to optimize the capture efficiency of magnetic particle at a targeted position through simulations performed using finite element based COMSOL Multiphysics software. Further, we study the effect of magnetic field, inlet velocity and particle size on the capture efficiency of magnetic particles transported in a fluidic channel through computational simulations. The obtained results through simulations are analyzed and calculated the capture efficiency for different magnetic field, inlet velocities and particle sizes. This study will help to design the better targeted drug delivery systems with improved capture efficiency at optimized values of inlet velocity, particle size and magnetic field.

MODEL DESCRIPTIONS

The mesh image of the geometry of magnetic particle transport in a fluidic channel under magnetic field applied through magnets placed outside the channel is shown in Fig. 1.

In this model, Navier-Stokes equation (equation 1) is taken for fluid flow and Newton’s equation (equation 7) for particle transport. The dominant drag and magnetophoretic force are considered which mainly affect the capture of magnetic particles under magnetic field.
Particle tracing module of finite element based COMSOL Multiphysics software is used to solve the non-linear Navier-Stokes equations. The mesh size is taken 10 µm to precisely observe the trajectories of magnetic particles. The fluid parameters used in the simulation are shown in Table 1.

Table 1: Fluid parameters used during simulation.

<table>
<thead>
<tr>
<th>Name</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dynamic viscosity</td>
<td>0.001002</td>
<td>Pa s</td>
</tr>
<tr>
<td>Density</td>
<td>1060</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Pressure</td>
<td>1</td>
<td>Pa</td>
</tr>
</tbody>
</table>

Equation for particle transport
\[
\frac{d(m\nu)}{dt} = F_t 
\]  
where F is Drag force, u is inlet velocity, \( \mu \) is viscosity and \( \rho \) is density of fluid.

Walls equation:
\[
u = 0 \text{ (no slip condition)}
\]  
Inlet equation:
\[
u = -u_0 n
\]  
Outlet equation:
\[
\left[\rho - \rho_f (\nabla u + (\nabla u)^T)\right] \n = -p_0 n
\]
where \( p_0 \leq \rho_0 \)

Equation for particle transport
\[
\frac{d(m\nu)}{dt} = F_t
\]

Magnetophoretic Force [21]:
\[
F_t = 2\pi r^2 \mu_r k \mu_0 H^2
\]
where \( F_t \) is magnetophoretic force, \( r \) is radius of particle, \( \mu_r \) is the relative permeability of magnet (\( \mu_r = 1 \)) and is assumed to be constant throughout the simulation, \( \mu_0 \) is the permeability in vacuum (\( \mu_0 = 4\pi \times 10^{-7} \) N/A²) and \( H \) is magnetic field vector (A/m).

Wall equation:
\[
\nu = \nu_c - 2 (u, \nu_c) n
\]
where \( \nu_c \) is the particle velocity when particle strikes at the wall of channel.

The Drag coefficients are defined as:
\[
C_D = \frac{2\pi r^2}{\rho U_{mean} L}
\]
where \( F_D \) is the drag force, \( \rho \) is the fluid’s density

\( U_{mean} \) is the mean velocity and \( L \) is the length of channel.

Drag Force Equation [20]:
\[
F = \nu \frac{\tau \rho u (u - v)}{\nu}
\]
\[
\tau = \frac{2\pi r^2}{\nu}
\]
Inlet equation:
\[
q = q_0, \nu = \nu_0
\]
Outlet Equation:
\[
\nu = \nu_c
\]
where \( \nu_c \) is the particle velocity when particle strikes at the wall of the channel.

These couple nonlinear equations (1 & 7) are solved using finite element based COMSOL software and observed results are presented below.

RESULT AND DISCUSSIONS

Effect of magnetic field on capture efficiency:
Fig. 2 shows the trajectories of magnetic particles flowing in a fluidic channel under the influence of different magnetic field. It is observed that 3, 4, and 5 number of particles are captured out of 10 at 2, 2.5 and 3 T magnetic field, respectively. Further, capture efficiency is calculated by using the formula:

\[
\text{Capture efficiency (\%) } = \frac{\text{number of captured particles}}{\text{total number of injected particles}} \times 100
\]

The value of capture efficiency, calculated using above formula (15), is found 30, 40 and 50 % at magnetic field 2, 2.5 and 3 T and shown in Table 2. This shows that capture efficiency increases as we increase the magnetic field. It is because that as we increase the magnetic field, the magnetophoretic force, experienced by the magnetic particles increases. This force is attractive in nature and mainly responsible to capture or attract the magnetic particles towards magnet (targeted region). Therefore, increasing the
magnetic field causes the large magnetophoretic force and results the enhancement in capture efficiency. Further, magnetic force equation (8) also states that magnetic attraction or force on a particle is proportional to the magnetic field strength. Hence the larger magnetic field applies the larger magnetic force on the particles and results the more accumulation of magnetic particles.

Effect of inlet velocity on capture efficiency:

Fig. 3 shows the trajectories of magnetic particles flowing in a fluidic channel at different inlet velocities. It is observed that 4, 3, and 2 number of particles is captured out of 10 at 15, 25 and 35 mm/s inlet velocities, respectively. This shows that captured number of particles decreases as we increase the inlet velocity. The value of capture efficiency, calculated using above formula (15), is found 40, 30 and 20 % at inlet velocity 15, 25 and 35 mm/s and shown in table 3. This shows that capture efficiency decreases as we increase the inlet velocities. Reduction in capture efficiency with inlet velocity is due to dominance of drag force at higher inlet velocities. The hydrodynamic force is proportional to fluid velocity and as fluid velocity increases, the hydrodynamic force increases, which overcome the magnetic force and make the particle free under the influence of attractive magnetic force and results the less accumulation of particles.

Effect of particle size on capture efficiency:

Fig. 4 shows the trajectory of magnetic particles flowing in a fluidic channel with different particle size. It is observed that the capture efficiency of magnetic particle increases as the size of magnetic particle increases. Simulation results show that 2, 3 and 5 out of 10 particles are captured for 100 nm, 1 µm, and 1.5 µm particle sizes, respectively. We again calculate the capture efficiency by using the formula mentioned in equation 15 and the value of capture efficiency is found 20, 30 and 50 % for 100 nm, 1 µm, and 1.5 µm particle sizes, respectively. This enhancement in capture efficiency by increasing the particle size is due to large magnetophoretic force experienced by large magnetic particles. As equation 8 shows that the magnetophoretic force is proportional to the cube of the radius of magnetic particles. So, the magnetophoretic force, which is attractive in nature and responsible to capture the magnetic particle, increases by increasing the particle size and results the enhanced capture efficiency for larger size particles.

CONCLUSION

In summary, the simulations are performed to study the capture efficiency of magnetic particles transported in a fluidic channel at different magnetic field, inlet velocity and particle size. The dominant magnetic and drag forces are considered in the equations used for simulations. The couple nonlinear Navier-Stokes equation for fluid flow and Newton’s second law equation for particle
transport are solved using finite element based COMSOL software. Results indicate that capture efficiency increase from 30 to 50 % as we increase the magnetic field from 2 to 3 Tesla, respectively. However, capture efficiency decreases from 40 to 20 % as we increase the inlet velocity from 15 to 35 mm/s, respectively. Furthermore, it is observed that capture efficiency increases from 20 to 50 % by increasing the particle size of magnetic particles from 100 nm to 1.5 μm, respectively. Enhancement in capture efficiency by increasing the magnetic field and particle size is due to enhanced magnetophoretic force, which is responsible to capture the magnetic particles. The obtained results can be utilized to optimize the parameters for performing the experiments related to magnetic drug targeting.

*Corresponding author: anurgdph@gmail.com, Tel.: +91-1744-233496

REFERENCES

BIOGRAPHY
Prakash Chandra received the B. Tech degree in Electronics and Instrumentation Engineering from West Bengal University of Technology. He is currently working toward the M. Tech degree in Instrumentation from NIT Kurukshetra. His research interest focuses on development of model and simulation work for targeted drug delivery using COMSOL Multiphysics Software. He has also expertise in the synthesis of nanoparticles and their characterization through XRD, SEM, UV Spectrometer and Photoluminescence.

Anurag Gaur received his Ph.D. degree from Indian Institute of Technology (I.I.T.) Roorkee in 2007. Currently, he is faculty at Department of Physics, National Institute of Technology, Kurukshetra. He has published about 85 research papers in peer reviewed journals and conference proceedings. He is also the reviewer of various AIP and Elsevier journals. He has guided many Ph.D. and M.Tech students for their dissertation work. His current research fields are Multiferroics, Functional Nanostructured Oxides Materials, Magnetoresitive Materials and Magnetic Drug Targeting.