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Analysis of Forces acting on Superparamagnetic beads in Fluid Medium in Gradient Magnetic Fields

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Abstract:

Superparamagnetic micro beads offer some attractive applications in biological and biomedical fields. Some of the important applications include manipulation and separation of cells, isolation of specific cells, active drug delivery, magnetic cell separation, separation of proteins, and application of mechanical forces to cells, etc. When non uniform magnetic field is applied on the beads, they form crystalline structures depending on the applied magnetic field, gradient of the magnetic field and the magnetic and drag forces acting on the beads. In the current work, focus has been on the analysis of the behavior of Superparamagnetic beads immersed in fluid medium when placed in non uniform gradient fields. A COMSOL Multiphysics model is developed in 2D with Magnetostatics, Fluid Dynamics and Moving Mesh Mode for predicting the motion of magnetizable beads in gradient fields, considering the effects of fluidic drag forces on the beads in the micro system. The model is developed based on the real experimental setup. Initial effort has been done in designing a 3D model to analyze the forces acting on the beads in various directions.

Keywords: Superparamagnetic beads, COMSOL Multiphysics, Magnetostatics, Fluid Dynamics, Moving Mesh, Video Spot Tracker, Image J.

Introduction:

Superparamagnetic beads have found wide use in both research and clinical medical diagnostic applications. There are two key properties of these beads. First, they are small in diameter to be colloidal, they remain dispersed due to random molecular bombardment of Brownian motion. They are of few micrometers in diameter and are made of a polystyrene matrix where iron oxide crystals are uniformly distributed. Secondly, they are Superparamagnetic. When a magnetic field is applied to superparamagnetic beads, the external magnetic field orients the magnetic dipoles of the iron oxide nanocrystals of which the beads are comprised, resulting in a magnetization of the bead, and an increase in the amplitude of the local field strength. Once the external field is removed, thermal energy randomizes the magnetic dipoles, removing any overall dipole, and effectively demagnetizing the beads. This behavior of superparamagnetic beads remains the same, regardless of the number of cycles to which the bead is subjected.

When Superparamagnetic beads are placed under the influence of a Centro-symmetric non uniform magnetic field in the presence of a fluid medium they arrange themselves in patterns which result in crystalline formation. The formation of structures, the spacing between the beads and the size of the structure formed mainly depends on the following

1. Strength of the field.
2. Gradient of the magnetic field.
3. Magnetic and drag forces acting on the beads

This work is focused towards understanding the forces which may act on Superparamagnetic beads in a gradient field, in which the magnetization of the beads also interact with one another. Such simple systems can give rise to high fidelity short and long range order due to the mobility of the magnetic components, and the patterns generated can be predicted using computational methods. In addition, the presence of magnetizable components that are not mobile can give rise to further variations in order, and act as templates if locally steep gradient fields are generated. The primary objective of this research is to build a COMSOL Multiphysics model that demonstrates the forces acting on Superparamagnetic beads, when non uniform magnetic field is applied to dispersed Superparamagnetic beads in a fluid field.

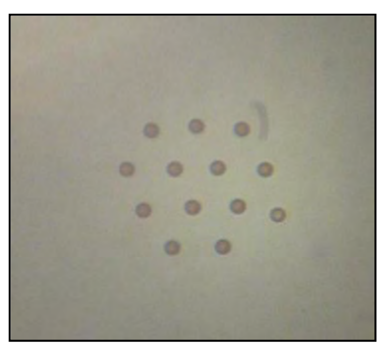


Figure 1: Crystalline Structure formed by 13 beads

Use of COMSOL Multiphysics:

The COMSOL Multiphysics is the primary application mode which can be used for coupling various multiphysics applications. The model in this work consists of the following coupled applications: Magnetostatics, Incompressible Navier Stokes, and Moving Mesh ALE. Using the Magnetostatics mode from Electromagnetism option, the steady state magnetic field medium is simulated. The output is shown in the form of surface plot showing the Magnetic Flux Density (B) and the surface contour plot showing the Magnetic Potential (z component). The Magnetic Force acting on the beads in both the x and y directions are calculated.

Using Incompressible Navier Stokes mode, the velocity that acts on the beads in both x and y direction due to the applied magnetic field is simulated using transient analysis. The magnetic field solution is stored as the initial solution in the model and the incompressible Navier stokes equation is solved. The Drag Force acting on the beads is calculated in both x and y directions.

The movements of the beads towards the magnetic tip are tracked down using the Moving Mesh (Arbitrary Lagrangian Eulerian), ALE mode. The values of the velocities the beads move with are given as the functional values from the Incompressible Navier Stokes mode. The results for the displacement of the beads in x and y directions are obtained. The results are stored in the form of the animation plot. Various other plots can be shown in the model like boundary plot, arrow plot, stream plot, cross section plot parameters. The results can be shown as Magnetic Field, Magnetization plots, Velocity Field etc.

Governing Equations:

Forces acting on beads:

The separation of magnetic micro particles suspended in a finite volume fluid involves the interaction of the Magnetic and Hydrodynamic forces.

a) Magnetic Force acting on the bead

The magnetic force acting on a dipole, $\vec{m}$ in an applied magnetic field $\vec{B}$ is

$$\vec{F} = (\vec{m}.\nabla)\vec{B} \qquad (1)$$

$$\vec{F} = \rho V(M_0.\nabla)B + \frac{V\chi_{bead}}{\mu_0}(\vec{B}.\nabla)\vec{B} \qquad (2)$$

Here $\vec{M}_0$ is the initial magnetization of the bead [Am^2/kg], V is the volume of the particle [m^3], χ_{bead} is the magnetic susceptibility of the bead, μ_0 is the permeability of the vacuum [H/m], and $\vec{B}$ is the applied magnetic field [T]. The susceptibility of the beads can be taken as $\chi_{bead} = (0.170 \pm 0.007)$.

b) Interaction Force acting between the beads

Along with the attraction forces between the magnetized beads, interaction forces between the beads are also present. According to equation (1), the term $\rho V(\vec{M}.\nabla)\vec{B}$ will be the interaction force acting between the beads. The equation (1) can be expanded into the component form as

$$\vec{F}_m = \rho V\begin{bmatrix} M_{0x}\frac{\partial B_x}{\partial x} + M_{0y}\frac{\partial B_x}{\partial y} + M_{0z}\frac{\partial B_x}{\partial z} \\ M_{0x}\frac{\partial B_y}{\partial x} + M_{0y}\frac{\partial B_y}{\partial y} + M_{0z}\frac{\partial B_y}{\partial z} \\ M_{0x}\frac{\partial B_z}{\partial x} + M_{0y}\frac{\partial B_z}{\partial y} + M_{0z}\frac{\partial B_z}{\partial z} \end{bmatrix} + \frac{V\chi_{bead}}{\mu_0}\begin{bmatrix} B_x\frac{\partial B_x}{\partial x} + B_y\frac{\partial B_x}{\partial y} + B_z\frac{\partial B_x}{\partial z} \\ B_x\frac{\partial B_y}{\partial x} + B_y\frac{\partial B_y}{\partial y} + B_z\frac{\partial B_y}{\partial z} \\ B_x\frac{\partial B_z}{\partial x} + B_y\frac{\partial B_z}{\partial y} + B_z\frac{\partial B_z}{\partial z} \end{bmatrix}$$

(3)

c) Drag Force acting on the beads

The third force that acts on the beads is the Stokes Force (or) the Drag Force $\vec{F}_{drag}$, due to the viscous drag exerted by the suspending medium on a moving bead. Stokes law explains the force needed to move a small sphere through a continuous, quiescent fluid at a certain velocity. The force depends on the radius of the sphere and the viscosity of the fluid. The system is modeled including no-slip boundaries on surfaces and the magnetic bead, and we expect to see wall effects. The equation for drag force is given as

$$F_{drag} = -6\pi\mu rv \qquad (4)$$

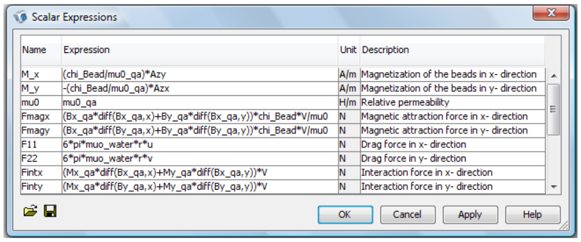
where μ is the dynamic viscosity of the fluid medium and v is the velocity of the bead.

The small diameter of the particles also causes them to reach equilibrium within the fluid very rapidly. The velocity ν of a particle following a step application of magnetic force is described by the differential equation (5)

$$\frac{dv}{dt} = \frac{F_{mag} - F_{drag}}{m_{par}} \qquad (5)$$

where m_{par} is the mass of the superparamagnetic bead.

The governing equations are transformed in to scalar expressions into the model using various variables formed with in the software. Figure 2 below shows various scalar expressions used in the model.



Name	Expression	Unit	Description
M_x	(chi_Bead/mu0_qa)*Azy	A/m	Magnetization of the beads in x- direction
M_y	-(chi_Bead/mu0_qa)*Azx	A/m	Magnetization of the beads in y- direction
mu0	mu0_qa	H/m	Relative permeability
Fmagx	(Bx_qa*diff(Bx_qa,x)+By_qa*diff(Bx_qa,y))*chi_Bead*V/mu0	N	Magnetic attraction force in x- direction
Fmagy	(Bx_qa*diff(By_qa,x)+By_qa*diff(By_qa,y))*chi_Bead*V/mu0	N	Magnetic attraction force in y- direction
F11	6*pi*muo_water*r*u	N	Drag force in x- direction
F22	6*pi*muo_water*r*v	N	Drag force in y- direction
Fintx	(Mx_qa*diff(Bx_qa,x)+My_qa*diff(Bx_qa,y))*V	N	Interaction force in x- direction
Finty	(Mx_qa*diff(By_qa,x)+My_qa*diff(By_qa,y))*V	N	Interaction force in y- direction

Figure 2: Scalar Expressions in the model

<u>Results</u>:

Magnetostatics mode is used for solving the magnetic field produced by the magnet, magnetic gradient acting on the beads, and the magnetic attraction and interaction forces acting on the beads. The bar is magnetized assuming that it has a remanent flux density of 1T. The constitutive relation used for magnetizing the bar is $B = \mu_0 \mu_r H + B_r$. The subdomain surrounding the magnet is considered as air.

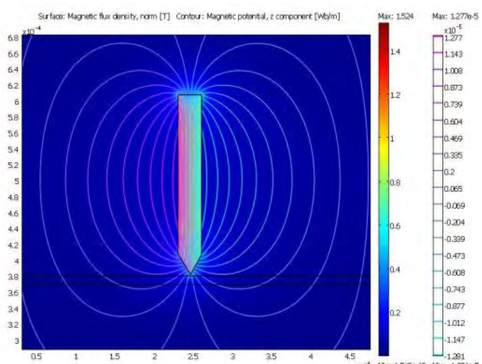


Figure 3: Variation of Magnetic Flux Density across the solenoid

Figure 3 shows the variation of magnetic flux density around the solenoid. It is evident from the surface plot that the magnetic flux density and decreases along the distance from the solenoid tip.

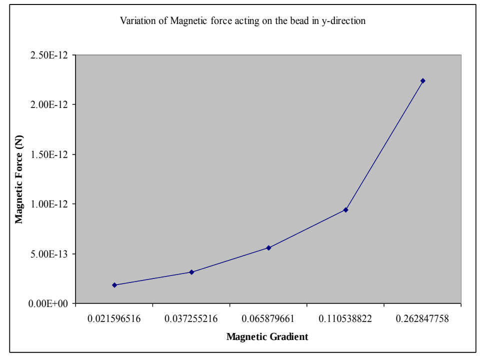


Figure 43: Variation of magnetic force with magnetic gradient

Figure 4 shows the variation of magnetic force with magnetic gradient. The value of magnetic gradient acting on the bead increases as the bead moves closer towards the solenoid tip and as a result the magnetic force acting of the beads increase.

The solution from the magnetostatics mode is stored and then the Incompressible Navier Stokes mode is solved for the fluidic drag forces acting on the beads. The forces are solved as transient analysis solver. The fluid considered in this simulation is water.

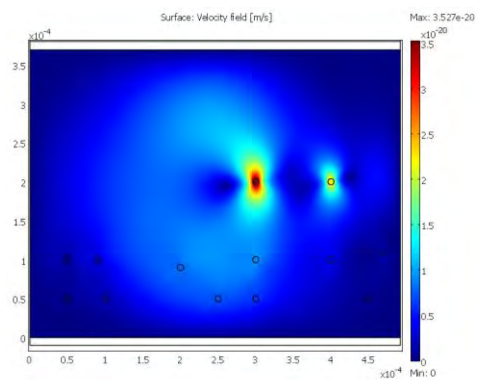


Figure 5: Surface plot showing the velocity field across the beads

Figure 5 shows the velocity field across the beads with which the beads move towards the solenoid. The beads far away from the magnetic tip experiences lower velocity field than the beads nearer to the magnetic tip. Variation of velocity field with the distance is showed in figure 6. The velocity acting on the beads increase as it moves towards the higher magnetic field.

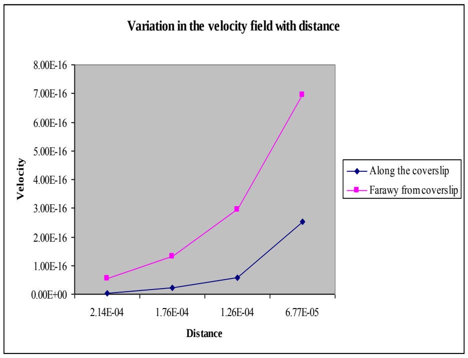


Figure 6: Variation of velocity acting on the beads along the distance from the magnetic tip

A low magnetic field is applied with the help of a permanent magnet placed beneath the cover slip on which the beads are placed randomly. The beads are packed between two cover slips filled in a finite fluid (water). The beads move towards the point of the application of the magnetic field (apex) and arrange themselves into crystalline structures depending on the magnetic gradient acting on the beads. Figure 7 below shows the experimental setup of the system.

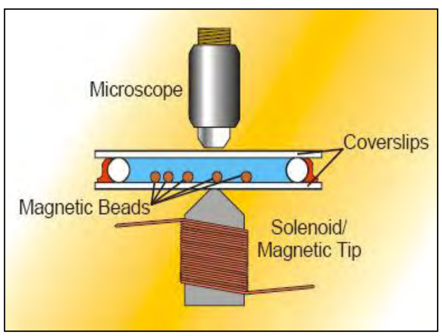


Figure 7: Experimental setup

Figure 8 below shows the sequence of steps in the formation of the structures.

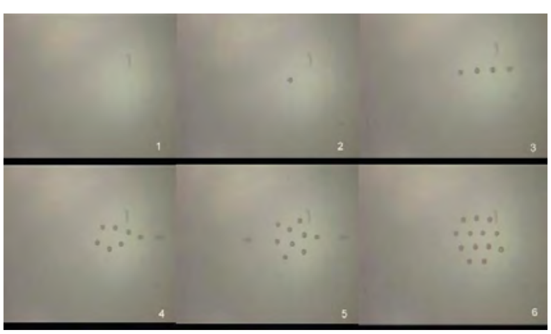


Figure 8: Sequence of steps in the formation of structures

From figure 8 it is observed that initially there are no beads, but as the magnetic gradient is acting on the beads, they start moving towards the center of the magnetic field (highest point). As each bead moves towards the highest point, the beads arrange themselves into structures that are stable. The final structure formed by the 13 beads is shown in 6th section in figure 8.

To extract the results from the movie obtained through the microscope Image J and video Spot Tracker software's are used. The movie is split into various frames depending on the accuracy, like 30 frames per second, 60 frames per second etc using any movie player (Quick Player). The displacement is obtained in pixels per frame. Figure 9 below shows the tracking of the beads using video spot tracker. Using Image J, pixels are converted into microns. The microscopic scale is imported into the Image J interface, and then the micron scale is converted into pixels. Thus this conversion will be used to convert the displacement in pixels to microns.

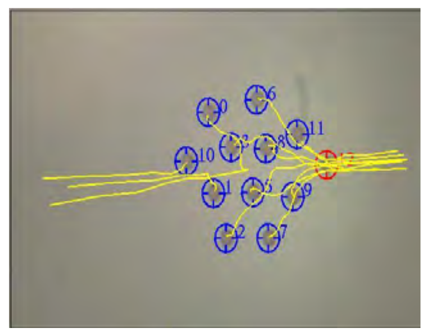


Figure 9: Tracking of beads

In order to show the displacement of the beads, two beads are considered. At equal intervals of time a surface plot is extracted at four different time intervals and using Image J all the four plots are added into a single plot. Figure 10 below shows the displacement of the beads and how they move towards the highest gradient position.

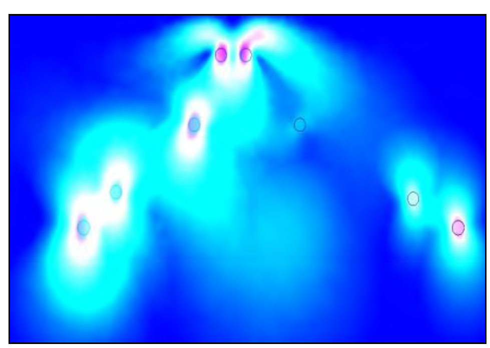


Figure 10: Displacement of two beads to a higher gradient point

Conclusion:

The model with 13 beads is successfully created. From the results it was found that the magnetization of the bead increases as it moves rapidly towards the magnetic tip depending on the magnetic gradient value. As the magnetization of the bead increase, the magnetic force acting on the bead also increases. After certain time, it is observed that the magnetization of the beads reached a saturated value, which depends on the material of the bead. As the beads come closer to each other, the interaction forces acting on the beads increases. Looking at the results it was evident that the velocity the bead moves with increases as it approaches the centre of the magnetic tip. As the velocities increased, the drag forces also increased.

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