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Finite Element Simulation, Characterization and Transportation of Magnetic Nanoparticles under the Impact of Magnetic Field in Blood Vessels

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Abstract

The drug delivery research based on magnetic particles has two major components. The first one discusses the preparation; characteristics and reaction of magnetic nanoparticles for the purpose of the transportation of the drug and the second part represents the drug delivery design for managing the dynamic of magnetic nano particles from injected positon to targeted area of vascular system. This study of the two parts of magnetic particles of drug delivery deals with preparation, Characterization, Synthesis and transportation of nano magnetic particles under the effect of external magnetic field in blood vessels. Co-precipitation method has been used for synthetization of nano crystalline Fe_3O_4 samples**.** The structural characterization and morphology of this sample has been done by using X-ray diffraction and Bruker D8 Advance X-ray diffractometer and Field Emission Scanning Electron Microscopy. After the study of preparation and characterization, the transportation of nano magnetic particles is explored under the effect of external magnetic field through a mathematical model. It is determined that the effect of external magnetic field through in constant fluid pressure, speed, distance of magnet and magnetic saturation is significantly affected by controlling the magnetic system that is required for an operative system of drug delivery. The non-dimensional partial differential equations are solved by using finite element method and they conclude that under the effect of external magnetic field, the

flow parameters presents a significant role for the investigation of the pattern of nano magnetic particles and blood.

Keywords: Characterization, Synthesis, Blood Vessels, Magnetic Nanoparticles, Magneto Hydrodynamics, FEM

1 INTRODUCTION

The method for transportation of drug into body of affected person in order to increase the drug consolidation in the affected parts of body as compared to the others parts is called targeted drug delivery by using magnetic nano particles [1-3]. In the study of fluid dynamic the dynamic of bio- magnetic fluid is a comparatively new area which is often used for the transmission of drug into the affected part of the body and also investigates the biological effects on flow under the influence magnetic field [4]. From last decades a well elaborated research work in biological fluid dynamics has been explored under the direct effect of magnetic field [5]. A lot of applications have suggested in the field of medical and bioengineering sciences in order to overcome the limitations of magnetic drug targeting. These applications include the development of magnetic traces, the research of magnetic devices for cell separation [6], the treatment of magnetic wounds or tumor of the cancers which caused magnetic hyperthermia [7-9], the reduction of bleeding during surgeries or the assistance of the blocking of the feeding vessels of the tumors of cancers and last but not the least as a drug carrier for the targeted transport of drug using nano magnetic participles [4, 10]. The drug delivery research based on magnetic particles has two major components. The first one discusses the characteristics and reaction of magnetic nanoparticles for the purpose of the delivery of the drug [11] and the second part represent the drug delivery design to control the dynamic of magnetic nano particles from injected positon to targeted area of vascular system. In this research we are researching both parts of magnetic particles drug delivery. In earlier methods, magnetic nano particles were seized by stagnant magnetic fields created by permanent magnets [12], or by superconducting magnets [13]. Further, it was searched that permanent magnetic field is not applicable effectively to target the deep parts inside body. Hence the sizes of magnetic nanoparticles ranging from nanometer to micrometer have become a searching material in the fields of magnetic recording and biological and medical applications [14]. The iron oxide having various products such as hematic (α-Fe2O3), maghemite (γ-Fe2O3) and magnetite (Fe3O4) are highly researchable magnetic nanoparticles. These magnetic nanoparticles are highly used for various purposes, for example, for carrying the drug [15], transport of drug [16, 17], for the treatment of cancer hyperthermia [18, 19], magnetic separation along with magnetic resonance imaging [20] and for exchanging of proton membrane and sensor [21].

The magnetic field along with superparamagnetic behavior at room temperature was highly responded by magnetic nanoparticles. Due to high saturated magnetization, the magnetic nanoparticles have become the most studied material in this field of biotechnology [22] . Moreover, the high biocompatibility and non-toxicity of magnetic nanoparticles are more useful in the field of biotechnology [23]. Further, in this research we are researching the synthesis and the characteristics of magnetic nanoparticles along with their transportation in blood vessels. For this purpose an extension is made in the mathematical model of bio-magnetic fluid dynamic represented by [24, 25]. In these models the Lorenz force that produced due to electric current of Magneto hydrodynamics [26], and magnetization of bio-magnetic fluid dynamic that agreeing with the Ferro-hydro-dynamics [27], were considered. A two dimensional axisymmetric mathematical model of blood flow and magnetic nano particles in a vessel is considered in this study. The flow is Newtonian, incompressible, laminar and fully developed in the blood vessel. A variable pressure and a consistent magnetic field are applied in the axial direction and perpendicular direction of blood flow respectively. In this study partial differential equation system, with suitable non-dimensional variables, is numerically solved by using finite element technique. Different values of parameters involved in this problem show that the obtained results of flow are significantly influenced by electric and magnetic forces. In the presence of variation of magnetic field, the axial velocity component extensively reduces. It is also concluded that for the formation of flow patterns, the electric forces and magnetic field gradient are the dominant factors. A comparison of results is also made by considering the effect of both magnetic and electromagnetic forces, without counting magnetic forces. The obtained results, deduced from the flow of bio magnetic fluid under the influence of applied magnetic field, are highly researched for more studies in the field of applied medical engineering.

2 THE MAGNETIC FIELD

MDT is one of the significant options of drug targeting. MDT helps to transport the drug at a targeted place with the support of magnetic field, by this way the transportation of the drug is enhanced on the targeted place for the purpose of reducing the side effects and toxicity in the normal tissues. Normally, magnetic material is based on iron, cobalt and ferrites which is also called Ferromagnetic Material and when the electric current flows through it, an electromotive force is produced as soon as this material flows in a magnetic field. And when the interaction of current with the magnetic field produces an electromagnetic force, as blood is an electrically conducting fluid, [28] it produces an electromagnetic force on the blood in the same way as external magnetic field applies. So in this study, nano magnetic particles made by iron oxide which move in blood in suspended form are basically

considered most important. Further these particles also enhance the electrical conductivity of blood under the influence of applied magnetic field and this electro motive force depends on the intensity of the magnetic flux and speed of moving particles [28]. In order to describe the motion of fluid and magnetic nanoparticles the model equations are coupled with Navier Stokes equations and laws of Maxwell for the magnetic field. The current density $\vec{J}$ is represented by Ohm′s law,

$$\vec{J} = \sigma(\vec{E} + \vec{V} \times \vec{B}) \tag{1}$$

Where, electric field intensity is $\vec{E}$, electrical conductivity is σ, magnetic flux intensity is $\vec{B}$ and velocity vector is $\vec{V}$. The momentum equation is defined as by considering electromagnetic force $\overrightarrow{F_{em}}$

$$\overrightarrow{F_{em}} = \vec{J} \times \vec{B} = \sigma\left(\vec{E} + \vec{V} \times \vec{B}\right) \times \vec{B} = -\sigma B^2 u \tag{2}$$

Where u is the axial velocity of the fluid? Maxwell equations for magneto static field and electromagnetic fields are $\nabla.\vec{B} = 0, \nabla \times \vec{H} = 0$, $\nabla \times \vec{B} = \mu_0 \vec{J}$, $\nabla \times \vec{E} = \frac{\partial \vec{B}}{\partial t}$

Where $\vec{H}$ is the strength of magnetic field.

The magnetic force which acts on magnetic nanoparticles is expressed as [29]

$$\vec{F}_M = \frac{\chi V_M}{\mu_0} \nabla(\vec{B}^2) \tag{3}$$

Here the susceptibility of the magnetic particles is χ , the free space permeability is μ_0, magnetic nanoparticles volume is V_M and density of magnetic flux is B . Also using $B = \mu_0 H$ in equation (3)

$$\vec{F}_M = \mu_0 V_M (\vec{M}.\nabla)\vec{H} \tag{4}$$

In the above equation; $\vec{M} = \chi\vec{H}$ is the magnetization feature of bio fluid, the impression of magnetic field on the flow is governed by magnetization. ∇ is the gradient operator. Numerous equations have been introduced in literature for magnetization property; and in this study, the linear formula that relates the magnetization to magnetic field strength and temperature is used [9]. On the scale of particle, it is assumed that external magnetic field is nearly constant for tiny particles. Moreover M may be substituted by the magnetization induced in a uniform external field. The radius of vessel near targeting area is very small. So the magnetic force across a blood vessel diameter is assumed as constant. The resisted forces on the

magnetic particles in the blood stream are produced due to blood flow which can be calculated by using stokes' expression.

$$\vec{F}_D = 6\pi\mu R_M(\vec{u} - \vec{v}) \tag{5}$$

Where μ is the viscosity of blood, R_M is the radius of the magnetic nanoparticle, u and v are velocities of blood and magnetic nanoparticles respectively. Hence in this study only those portions of blood vessels are considered useful which oriented perpendicularly to the direction of the magnetization. For this purpose the intensity of magnetic field in the direction of magnetization for the cylindrical magnet is given by [9]

$$H_y = \frac{C_1 a^2}{y^2} \tag{6}$$

Where 'a' is the radius of cylindrical magnet and $C_1 = 500000 Am^{-1}$, oz is the direction of magnetization which is oriented perpendicular to the direction of blood vessel feeding the tumor as shown in Fig 1.

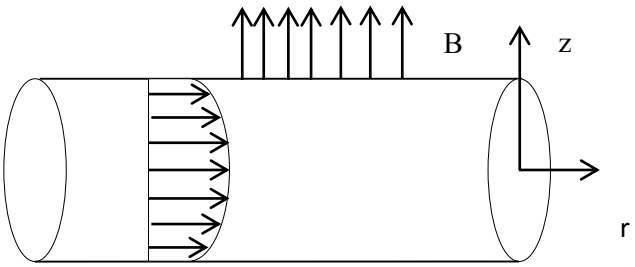

Figure 1 geometry of flow in blood vessel

3. MATHEMATICAL MODEL

The dynamic of blood and magnetic particles is represented by using mass and momentum conservation equations. Therefore, it is considered that the flow occur in axial direction under the impact of external magnetic field. So in this study blood is considered as laminar axisymmetric flow of a viscous, homogeneous, and incompressible Newtonian fluid in the cylindrical blood vessel.

The dynamic equations of momentum and mass for the blood and magnetic particles in the cylindrical polar coordinates are given respectively by the equations given under

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho}\frac{\partial P}{\partial z} + \nu\left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r}\right) + \frac{KN}{\rho}(v-u) - \frac{\sigma B^2 u}{\rho} \tag{7}$$

$$m\frac{\partial v}{\partial t} = \mu_0 V_M(\mathrm{M}\nabla\mathrm{H})_z + 6\pi\mu R_M(u-v) \tag{8}$$

Where v and u are the velocities of magnetic nanoparticles and blood respectively. ρ is the density of blood, μ is the dynamic viscosity of fluid, ν is the kinematic viscosity, $\frac{\partial P}{\partial z}$ is the pressure gradient, N is number density of suspended nanoparticles, K is stoke,s coefficient , m is mass of magnetic nanoparticles, σ represents the electric conductivity and at the end t is time parameter. Here the pressure gradient is independent of radial coordinate and eventually the pressure gradient appearing in (8), and it has been taken from Burton [30] .

$$-\frac{\partial p}{\partial z} = A_0 + A_1 cos\omega t \tag{9}$$

Where, constant amplitude of pressure gradient is A_0, A_1 is the amplitude of the pulsatile component which gives rise to diastolic and systolic pressure.
The initial and boundary conditions given under the points

i.It is supposed that no flow occurs when system is at rest.

$$u = v = 0 \quad at\ t = 0 \tag{10}$$
$$\frac{\partial u}{\partial r} = 0 \ at \quad t = 0$$

ii.Velocity on the vessel wall is taken as

$$u = v = 0\ at\ r = R \tag{11}$$

Where R is the radius of the vessel.

4 TRANSFORMATION OF EQUATIONS

Transformation equations are used to reduce the computational complexity. The mathematical model for this purpose is rescaled by using the following transformation equations.

$$r^* = \frac{r}{R}, z^* = \frac{z}{R}, y^* = \frac{y}{R}, t^* = \frac{t\mu}{\rho R^2}, v^* = \frac{vR}{\nu}, u^* = \frac{uR}{\nu}, H^* = \frac{H}{H_0} \tag{12}$$

Where, kinematic viscosity is $\nu = \frac{\mu}{\rho}$ and intensity of magnetic field is H_0 at the surface of the magnet. By applying Transformation equation (12) and dropping *, the governing equations (7-8) become:

$$\frac{\partial u}{\partial t} = (A_0 + A_1 cos\omega t) + \nu\left(\frac{\partial^2 u}{\partial r^2} + \frac{1}{\bar{r}}\frac{\partial u}{\partial r}\right) + A_3(v-u) - Ha^2 u \tag{13}$$

$$\frac{\partial v}{\partial t} = A_1(\nabla \mathrm{H})_z + A_2(u - v) \tag{14}$$

Where, $A_3 = \frac{NKR^2}{\rho\nu}$,$A_2 = \frac{KR^2}{m\nu}$,$A_1 = \frac{\mu_0 V_M H_0 M R^2}{m\nu}$,$K = 6\pi\mu R_M$ is the Stokes Coefficient. Ha is Hartmann number. The initial and boundary equation becomes $u = v = \frac{\partial u}{\partial \bar{t}} = 0$ at $t = 0$

$$u = v = 0 \quad \text{at} \quad r = 1$$

Finite element method is used to solve the non-dimensional governing equations (13) and (14) with initial and boundary conditions. For space discretization 0.01 is consider as mesh spacing. The obtained time dependent system of equations is solved by finite element method with mesh spacing of 0.002, 0.004, 0.006 and 0.008.

Table 1: Symbols, constant with their typical values

Symbol	variable	units	Typical value
u	Velocity of blood	m/s	*
v	Velocity of MNP	m/s	*
P	Pressure	Pa	*
μ	Blood dynamic viscosity	Kg/ms	0.035
R_M	radius of MNP	nm	$100*10^{-9}$
υ	kinematic viscosity	m^2/s	μ/ρ_0
R	radius of capillary	m	$3*10^{-6}$
H	Magnetic intensity	A/m	*
μ_o	permeability of free space	H/m	$6\pi * 10^{-7}$
V_M	Volume of MNP	m^3	$4/3\pi R_M^3$
m	Mass of MNP	kg	$\rho_p V_M$
ρ	density of blood	Kg/m^3	1050
ρ_p	density of MNP	Kg/m^3	$5.1*10^3$
T	time	s	*
M	Magnetization	N/m^2T	4.5*10^3

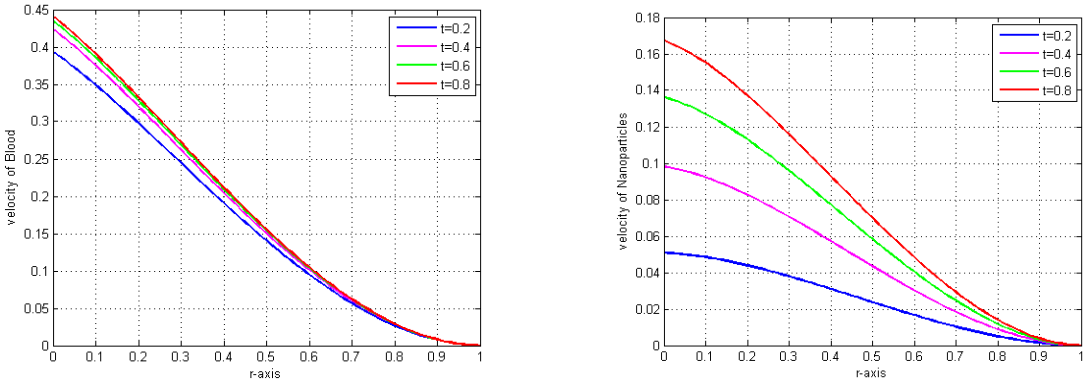

Figure 4 Axial Velocity profiles of blood and magnetic nanoparticles in blood vessel for different time (without magnetic forces)

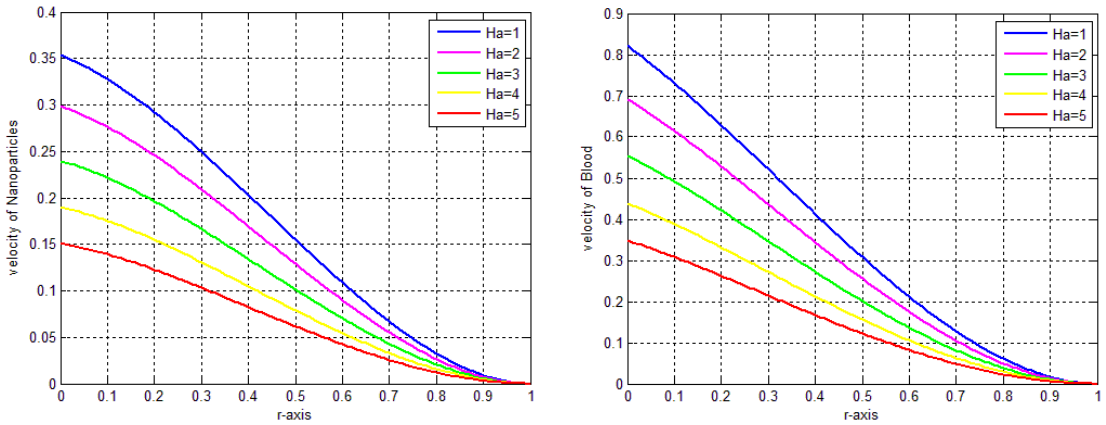

Figure 5 Axial Velocity profiles of blood and nanoparticles in blood vessel for different Ha

5. RESULTS AND DISCUSSION

The axial velocity profiles of magnetic nano particles and blood at different axial locations are represented by figure 4. The all axial profiles of velocity have a same trend and show reduction from their maximum at the axis and finally become close to zero on wall surface.

It is being observed that owing to the unsteady nature of flow, the velocity profiles get rise as time march towards the axis as compared to the surrounding area of the wall surface.

Figures 4 also show pulsatile dependency of both blood and particles with time and get maximum velocity when time is 0.8s. The trends also show that moving path of magnetic nano particles and blood is same but the movement of magnetic nanoparticles is fewer in contrast with the movement of blood due to retardation and drag forces. The magnetic nanoparticles and blood have maximum velocity at the axis respectively as 0.4407 and 0.1673.

The velocity profiles of blood and magnetic nanoparticles for various axial locations with Hartmann number ranges from 1 to 5 are showed in figure 5. Through these figures one can notice that significantly the reduction in the velocity of blood and magnetic nanoparticles due to presence of magnetic forces. It is also being noted that an increase in the Hartmann number causes the decrease in the trends. As a result the axial velocity of blood ranges from 1.0284 to 0.4407 as Ha ranges from 1 to 5. It may be due to fact that when magnetic field is applied to the blood, the charged particles of blood and magnetic particles receive a rotational force due to the action of the magnetization which causes them to rotate under the effect of magnetic field.
The magnetic nanoparticles and red blood cells suspended in the plasma fluid due to this action of magnetization and resultantly it increases the concentration on magnetic particles and in this way the internal viscosity of blood increases leading to the decrease in the velocity of axial flow.

Since the Lorentz force act against the flow of magnetic nanoparticles and blood as magnetic field applied, due to this factor the reduction in axial profiles will occur by increasing the magnetic field. Correspondingly, the reduction in velocity of magnetic nano particles ranges from 0.3862 to 0.1673 as by increasing Ha ranges from1 to 5, respectively as shown in (Fig. 5). From figure 5, It is also observed that when Ha=1 the blood velocity (1.0284) is greater as compared to the velocity of magnetic nanoparticles (0.3862). This will happen because the magnetic nanoparticles move along with blood and face Lorentz force when passes from the magnetic field. Furthermore, this force behaves like a resistive drag force that reduces the normal flow of magnetic nano particles due to torque of magnetization which applied on magnetic nano particles. On the other hand, Lorentz force acts against the movement of magnetic nano particles and blood more powerfully as increasing the Hartmann number and hence the velocity decrease further in axial direction.

6 METHOD OF SYNTHESIS

Co-precipitation method has been used for synthetization of *nano crystalline* Fe_3O_4 samples. In this method, 3.0g of ferric chloride ($FeCl_3 \cdot 6H_2O$, 98%) and 1.5g of ferrous chloride hexahydrate ($FeCl_2 \cdot 4H_2O$, 99%) are dissolved in de-ionized water of 100 ml at 60 °C. After mechanical stirring for 30 minutes, the color of this mixture becomes red (wine color). After this precipitated 10 ml of 25 wt% NH_4OH is added to the solution under constant stirring and maintains the temperature of the solution at 80 °C till the pH of the solution becomes ~7.0. This manages the construction of precipitate of black color and subsequently the temperature of this is sustained at 80 °C for 2 hours. After this, the precipitate is allowed to settle down and then filtered [31]. In order to remove all impure ions, the developed precipitate is acetoned 5–10

times and washed by using de-ionized water. The composed magnetic nanoparticles are dried in a vacuum with 100 °C for 12 hours to get nanoparticles of Fe_3O_4.

6.1 Characterization

The structural characterization of the sample is done by using X-ray diffraction and Bruker's D8 Advance X-ray diffractometer (XRD), the diffractogram is noted by using time step 1 second and interval step as 0.02º between 2θ ranges of 20º - 80º at room temperature. The classic KBr pellet technique is used to identify the functional groups by FTIR analysis and it is performed on Nicolet iS50 spectrometer. The spectra is noted in a wave number ranging from 400-4000 cm^{-1} in transmission way with 32 scans and 4 cm^{-1} of resolution. The chemical composition and morphology are studied by using FESEM, Zeiss-LEO Model 1530.

6.2 Experimental Results and discussion

The X-ray diffractometer is used for characterization of crystalline structure of the Fe_3O_4 nanoparticles. Figure 1 represents that the values of d-spacing for important peaks match with the data from (JCPDS 19-029) very well for Fe_3O_4. The diffraction peaks at 2θ = 30.13°, 35.48°, 43.12° and 65.81° can be allocated respectively to the (2 2 0), (3 1 1), (4 0 0) and (4 4 0) planes, , which shows that pure Fe_3O_4 is used for formation of cubic spinel crystal [32].

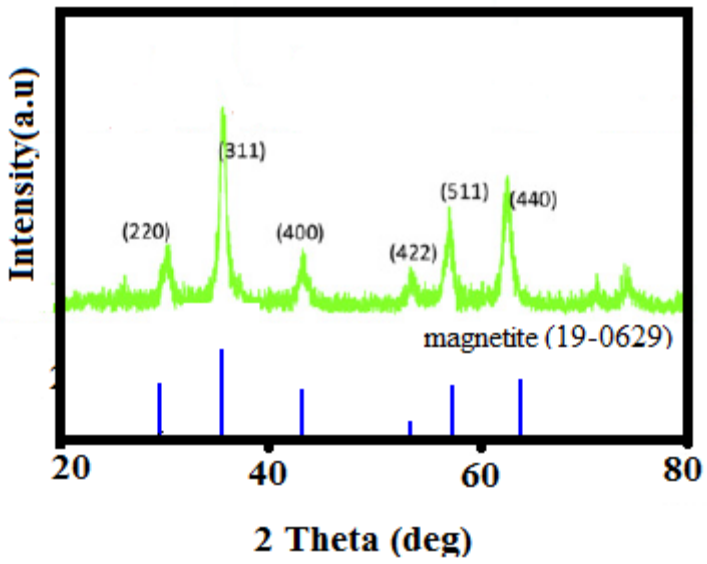

Fig. 1: XRD patterns of the magnetite nanoparticles

Figure 2 represents the FTIR spectra of the magnetite nanoparticles. For the magnetites, the peak at 643 cm^{-1} corresponds to the vibration of the Fe-O bonds. Further, the peaks at 1667 and 3413 cm^{-1} may be attributed to the stretching vibration of the hydroxyl groups on the surface of the magnetite nanoparticles [14].

The surface morphology of the synthesized Fe_3O_4 samples has been studied by FESEM technique. The FESEM micrographs shown in Fig. 3 indicate that mostly particles are in polyhedral shape, almost uniform and nano-sized in the 100 nm. Furthermore, FESEM images show the agglomeration of nanoparticles. This is due to presence of magnetic interactions among the particles [31].

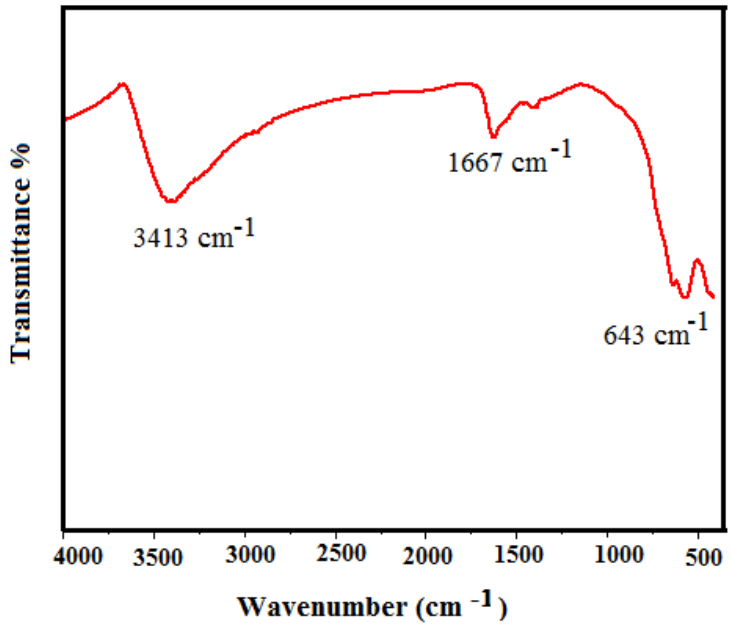

Fig. 2. FTIR spectra of the magnetic nanoparticle

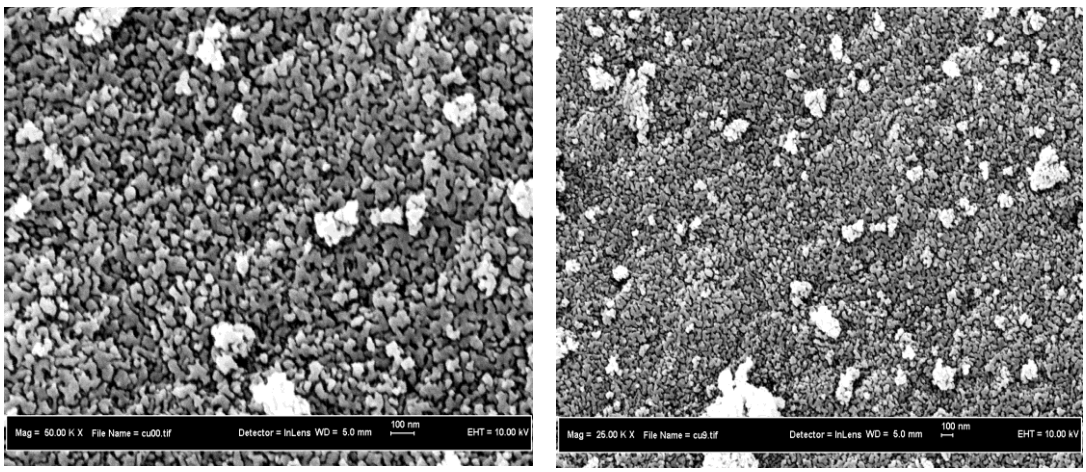

Fig. 3. FESEM images of the magnetic nanoparticles having 100 nm radius

7 CONCLUSION

In this study synthetization, characterization and transportation of magnetic nano particles in blood vessel are investigated. Co-precipitation method is used for synthetization of nano crystalline Fe_3O_4 samples and developing precipitate is washed by using de-ionized water in order to remove all impure ions. The structural characterization and morphology are done by using XRD and FESEM. Furthermore, in this study a comprehensive mathematical model is presented to explore the transportation of these magnetic nanoparticles under the impact of strong magnetic field in blood vessels. In this model the basic set of Maxwell's equations have taken along with momentum and mass equations. A finite element approach is applied to solve partial differential equations numerically. The results show that transportation of magnetic nano particles and blood is significantly reduced under the impact of magnetic field. It may be observed that in practical circumstances, a significantly weaker magnetic field can be used for drug targeting. Due to this fact the magnetic particles increase the susceptibility of magnetic field by insufficient orders of magnetic particles, and as a result the effects of magnetisation force become stronger. The mathematical model in this study may be convenient for designing and optimization of such systems. Similar simulations may be carried out for investigation of behaviour of magnetic nanoparticles in multi branching blood vessels.

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