Steering the Drug Release of Smart Magnetic Self-Assembled Nano Micelles in an Internal Thoracic Artery Flow for Breast Cancer Therapy

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Abstract

Magnetic drug targeting (MDT) is one of the most modern techniques in cancer therapy for its ability to reduce the side effects of chemotherapy experienced by systemic administration. In this study, a comprehensive mathematical model has been developed to predict the drug particle trajectories of anticancer dasatinib magnetic nanomicelles (DAS-MNM) released in an internal thoracic artery (ITA) blood flow for breast cancer therapy. Several factors are investigated in regard to the efficiency of MDT through the ITA, including magnetic field strength (MFS), relative magnetic permeability, magnet size, drug particle size, and, initial position of drug particle. The drug particle trajectory results confirmed the successful MDT using an external magnetic field with a capture efficiency of more than 90%, through the accumulation of a wide range of particle sizes of DAS-MNM close to the external magnetic field source at the arterial wall than in other positions. Moreover, the results showed that the number of trapped particles increased with increasing both MFS and drug particle diameter within the target tissue, while the drug particle permeability does not have a considerable effect on the particle retention. In addition, for achieving a successful drug/cargo delivery through the arteries, the magnetic field, the particle size, and initial release locations should be adjusted simultaneously. The present work offers insights into the critical factors in MDT with a significant impact on breast cancer therapy, tissue engineering, and regenerative medicine.

1. Introduction

Controlled drug release using magnetic nanoparticles (MNPs) is getting great interest in cancer therapy due to its ability to reduce the side effects of chemotherapy. Targeted treatment within the boundaries of the affected area without damaging healthy cells is a desirable object [1]; [2]; [3]. To improve the chance of successful therapy with reduced side effects, various methods of passive and active drug delivery are demonstrated [4]; [5]; [6]. In passive targeting, it is important to take into account the specific properties of the tumor, such as the nanoparticle size, and surface characteristic of the diseased area [7]; [8]. There are a number of different techniques that have been studied to actively target such as pH-sensitive particles [9], encapsulated ligand [10], ultrasound-guided nanoparticles [11], and magnetic fields [12].

Magnetic drug targeting (MDT) system is considered to be one of the most promising drug delivery systems for delivering therapeutic agents to tumors and other disease sites [13]; [14]. Magnetic nanoparticle (MNP) are appealing as drug delivery systems because of their magnetic cores, ability to load drugs, and biochemical properties. Further, the trajectory of MNPs could be controlled by creating internal or external magnetic fields with permanent magnets and coils [15]; [16].

Several parameters have also been examined in an effort to elucidate how the drug particle cluster performance for MDT through arteries can be influenced, like a magnetic field, particle size, bulk flow velocity, and velocity profile. It was established that the particle trapping decreases with increases in the bulk flow velocity, and the velocity profile does not significantly affect particle retention. Moreover, an enhancement in the particle capture efficiency is observed with increasing magnetic field strength (MFS)
and drug particle diameter in small vessels with low blood flow. Numerous mathematical models have been developed on the magnetically guided drug delivery systems to investigate the efficacy of MDT. Zhang et al. (2020), developed a mathematical model of MDT using ANSYS software to predict the drug particle trajectories by an external magnetic field for atherosclerosis therapy. The magnetic field generated by the wire contains a current and wire shape are the main parameters for drug delivery to the target. A smart haptic guidance scheme to guide a number of magnetic nanoparticles (MNPs) using forbidden area virtual fixtures and a haptic multi-particle rendering scheme was proposed by. They found that the targeting efficiency was greatly improved using the forbidden virtual fixture region and the proposed haptic rendering of MNPs.

Patronis et al. (2018), implemented a promising work on drug management in the human body using magnetic fields that acted on nanoparticles made of paramagnetic materials. They developed a computational model to simulate the magnetic targeting of a drug in certain geometry of a patient's brain by controlling paramagnetic nanomicelles using an external magnetic field. The model connects the dynamics of spherical drug particles with hydrodynamic modeling of the lattice-Boltzmann taking into account the body's strength, diffusion and dipole interactions.

Jungwon et al. (2017), proposed a novel electro-magnetic push-and-focus spherical particles (SPP) actuation system to a deep tumor region and investigated the effects of the SPP in realistic blood vessels with a maximum length of about 10–12 cm, the simulation results show that the 500 nm SPPs can be concentrated on a target tumor region with up to 97.9% efficiency.

In this study, a computational drug delivery model in a COMSOL environment is performed, to predict the particle trajectories of DAS anticancer drug encapsulated in nanomagnetic self-assembled micelles released in an internal thoracic artery flow.

2. Drug Delivery Model

2.1. Paradigm

The internal thoracic artery (ITA) with an external permanent magnet was represented using a two-dimensional model. Figure 1a shows the ITA and its branches in the human body. The schematic depiction for the MDT model is illustrated in Fig. 1b, an external permanent magnet is implanted at the target drug release site, which generates a magnetic field that attracts the MNP. The ITA as a blood vessel, is an artery that supplies the anterior chest wall and the breasts. The left internal thoracic artery (LITA) and right internal thoracic artery (RITA) originated directly from the subclavian artery. The length of LITA is different from 159 to 220 mm, with a mean of 182.60 mm from the origin to the end point, and a diameter of 2.31 ± 0.70 mm. The RITA varied from 150 to 231 mm, with a mean length of 185 mm and a diameter 1.98 ± 0.04 mm.
Dasatinib (DAS) was selected as a breast anticancer drug encapsulated in nano magnetic self-assembled micelles as reported in our previously reported work \[24; 25\]. Briefly, the magnetite nanomicelles (MNMs) were prepared using the co-precipitation technique. The magnetite nanoparticle was prepared by dissolved 2.2 g of FeCl\(_2\).4H\(_2\)O and 5.8 g of FeCl\(_3\).6H\(_2\)O in 200 mL of distilled water at room temperature. Then, the solution was heated to 70 °C and 10 mL of NH\(_3\)OH (30%) was added rapidly under higher stirring to produce a black precipitate. After that, 5 mL of hexane was added to 20 mg of magnetite nanoparticles, the magnetite solution was added dropwise to 50 mL of distilled water containing 100 mg of zein-lactoferrin micelles. The MNM was formed by sonication the mixture for 30 min at 50 °C under nitrogen flow. DAS is a highly hydrophobic anti-cancer drug, the solvent evaporation method was used to encapsulate DAS into the inner MNM core. The DAS was dissolved in ethanol (1 mg/mL) and added slowly to 50 mL of MNM solution (2 mg/mL), Afterward, it was stirred at a moderate magnetic field overnight to let the ethanol evaporate and encapsulate the DAS into the inner hydrophobic core of the zein-lactoferrin micelles [24]. A model has been developed to simulate DAS-MNM released into the ITA blood vessels and trajectory to specific targets by an external magnetic field.

### 2.2. Governing Equations

To simulate DAS-MNM delivery at the target sites, the blood flow, magnetic static field, and particle tracking domains were used in this model. The laminar blood flow and far from the heart are considered. Navier–Stokes continuity and momentum equations (Equations (1) and (2)) are used to derive the blood velocity and pressure profiles into ITA [8].

\[
\rho \nabla \cdot \bar{u} = 0 \tag{1}
\]

\[
\rho (\bar{u} \cdot \nabla) \bar{u} = -\nabla P + \mu \nabla^2 \bar{u} + \vec{F} \tag{2}
\]

where \(\bar{u} \) (m/s) refers to the velocity vector; \(\rho \) (kg/m\(^3\)) is the blood density; \(\mu \) (Pa•s) is blood dynamic viscosity; \(P \) (Pa) is the pressure; and \(\vec{F} \) (N/m\(^3\)) is the external forces. Since the model deals with a low Reynolds number blood flow, the inertial term can be ignored in Eq. (2).

The rheology of blood flow can be explained by several models. Johnson and colleagues investigated one Newtonian blood flow model and five non-Newtonian blood viscosity models simulation [27]. It was established that the power-law model is satisfactory for fitting the experimental results over strain rates range \((\dot{\gamma}), 0.1 < \dot{\gamma} < 1000 \text{ s}^{-1}\). Additionally, many other blood models behaviors summarizes the power-law behavior at low strain rates and Newtonian behavior at high strain rates [27]. Thus, the power-law model was used to define the rheology of blood in our model [28].

\[
\eta = \lambda \left| \dot{\gamma} \right|^n \left( \dot{\gamma} \right)^{-1} \tag{3}
\]
\[ \lambda(\dot{\gamma}) = \eta_\infty + \Delta \eta \exp \left( - \left( 1 + \frac{\left| \dot{\gamma} \right|}{a} \right) \exp \left( \frac{-b}{\left| \dot{\gamma} \right|} \right) \right) \] (4)

\[ n(\dot{\gamma}) = n_\infty + \Delta n \exp \left( - \left( 1 + \frac{\left| \dot{\gamma} \right|}{c} \right) \exp \left( \frac{-d}{\left| \dot{\gamma} \right|} \right) \right) \] (5)

where \( \left| \dot{\gamma} \right| \) is the strain rate magnitude. The parameters values used in our model were quoted from the work of Ballyk and co-workers [28]: \( \eta_\infty = 0.0035 \text{ kg/(m.s)} \), \( \Delta \eta = 0.025 \text{ kg/(m.s)} \), \( a = 50 \text{ s}^{-1} \), \( b = 3 \text{ s}^{-1} \), \( n_\infty = 1 \), \( \Delta n = 0.45 \), \( c = 50 \text{ s}^{-1} \), and \( d = 4 \text{ s}^{-1} \).

The magnetic field surrounding a permanent magnet is defined by the following Equations [29].

Ampere-Maxwell equation for static magnetic field:
\[ \nabla \times H = J \] (6)

Gauss's law for the magnetic flux density:
\[ \nabla \cdot B = 0 \] (7)

The magnetic flux density in different domains can be described by the relation between \( H \) and \( B \).
\[ \nabla \cdot \left( \mu_o \mu_r (H + B) \right) = 0 \] (8)

where \( H \text{ (A/m)} \) is magnetic field strength; and \( B \text{ (A/m)} \) is the magnetization of the magnet. \( \mu_o \) and \( \mu_r \) are the relative magnetic permeability of free space and fluid respectively.

In the particles tracing domain, there are a number of factors that have an impact on the DAS-MNM motion including magnetophoretic force, viscous force, inertial force, gravitational force, Brownian motion, and interparticle interaction. It might be possible to synthesize the particles in a way to prevent interparticle interactions that would lead to agglomeration [30]. Since the particle diameters are greater than 50 (nm), Brownian motion is neglected [8]. Furlani and Ng [31] observed that magnetization and viscous forces are the dominant forces in diluted particle suspensions. Newton's second law is considered for the particle tracing domain as shown by Eq. (9) [29].

\[ \frac{d(m_p \vec{V})}{dt} = \sum \vec{F} \] (9)

where \( m_p \) is the mass of particles and \( \vec{V} \) is particle velocity. \( F \) is the sum of magnetophoretic and viscous forces acting on the particles.
In presence of an external magnetic field, Ferro particles are magnetized and steered towards a magnet. From Eq. (10) can determine the resultant magnetophoretic force [32].

$$\vec{F}_{MP} = \frac{\pi}{4} d_p^3 \mu_0 \mu_r K \vec{\nabla} H^2$$ (10)

$$K = \frac{\mu_p - \mu_r}{\mu_p + 2 \mu_r}$$ (11)

Where $d_p$ is particle diameter; $\mu_p$ is particles permeability.

Stokes drag model is utilized to estimate the drag force acting on particles. [33].

$$Re_r = \frac{\rho |\vec{u} - \vec{V}| d_p}{\mu}$$ (12)

$$\vec{F}_D = \frac{\rho_p d_p^2}{18 \mu} m_p (\vec{u} - \vec{V})$$ (13)

where $\rho$ (kg/m$^3$) is the density of blood; $\mu$ (Pa·s) is blood viscosity; $d_p$ (m), $\rho_p$ (kg/m$^3$), $m_p$ (kg), indicate particles diameter, density, and mass respectively; $\vec{u}$ (m/s) is blood velocity, and $\vec{V}$ (m/s) is particles velocity.

According to Calandrini et al., capture efficiency is assessed using Eq. (14), [34].

$$\eta_C = \frac{N_{in} - N_{out}}{N_{in}}$$ (14)

where $\eta_C$ is the capture efficiency; $N_{in}$ is the total number of DAS-MNM injected; and $N_{out}$ is the total number of MNMs swept away.

The numerator in Eq. (14) is a good indicator of the MDT's ability in delivering DAS-MNM, which equates to the number of DAS-MNM delivered to the target zone.

### 2.3. Geometry Meshing and Numerical Procedures

To mimic the truthful flow conditions of ITAs, a well-defined geometry and a fairly simple approach were utilized. Figure 2 illustrates three different domains were generated with various numerical grids. The maximum element size for numerical free triangular mesh in magnetic field domain (1), external magnet domain (2), and blood vessel domain (3) were 0.25, 0.08, and 0.04 mm, respectively. The geometry included only one main inlet ($D_{inlet} \approx 3$ mm) and eight outlets ($D_{outlet} \approx 2–1.5$ mm). The magnetic field and a velocity profile in the artery are the two characteristics of the model that describe blood flow during magnetic drug targeting.
In this model, all calculations were implemented by commercial software COMSOL Multiphysics® 6.0. Initially, the model required several interfaces physics to be applied:

1. CFD module involving sophisticated blood flow models.
2. AC/DC module for generating magnetic fields.
3. Particle trajectories module

Through the COMSOL Multiphysics, it is possible to create a 2D geometry of the artery and an external magnet implanted as shown in Fig. 2. Equations (1–14) were used to simulate non-Newtonian blood flow, magnetic fields, and particle trajectories. In this study, 5000 particles of DAS-M&M are released and their retention with the magnetic field is studied. Simulators have been applied to the magnetization domains using the stationary solver, and the derived values have been used as well-known values in the time-dependent simulation. Table 1 shows a detailed of the material properties used in the simulation.

<table>
<thead>
<tr>
<th>Property</th>
<th>Blood</th>
<th>DAS-MNM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m³)</td>
<td>1060</td>
<td>5230</td>
</tr>
<tr>
<td>Viscosity (Pa.s)</td>
<td>0.0035</td>
<td>—</td>
</tr>
<tr>
<td>DAS-MNM particle size (nm)</td>
<td>—</td>
<td>100–500</td>
</tr>
<tr>
<td>Relative magnetic permeability (A/m)</td>
<td>1.0</td>
<td>3.0–15.0</td>
</tr>
<tr>
<td>Magnetic field strength (T)</td>
<td>—</td>
<td>0.5–2.0</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>293.15</td>
<td>—</td>
</tr>
</tbody>
</table>

### 3. Results And Discussion

#### 3.1. CFD Blood Flow

Following a stationary solver of the magnetic field, time-depending simulations of the arterial blood flow were performed using the Navier-Stokes equation. Matsuo and co-workers [35] analyzed the physiological waveform blood flow utilizing a Doppler flowmeter catheter. Figure 3 (top) illustrates the blood velocity for 5 s, the data was extracted digitally and fit using a 9-degree polynomial. During systole, blood flows slowly forward (S wave) and during diastole, it flows rapidly forward (D wave). It can be seen that the peak of the S wave is just below half of the peak of the D wave. Each cardiac cycle can be divided into seven parts of a second according to the acceleration and slowness of the blood flow velocity. Starting at (a) t = 0, is the point before the blood slows down, followed by the maximum reverse velocity at point (b) t = 0.14 s. The peak of the S wave is at point (c) t = 0.34 s, the midpoint of the acceleration phase at (d) t = 0.45 s, and the (g) t = 0.87 s is the maximum forward velocity point of the D wave peak [35].
The contours plot of blood velocities is illustrated in Fig. 3 (bottom), the red arrow marks the main inlet with a 3.0 mm diameter. From right to left, the eight branches outer diameters are 2.0, 1.75, 1.75, 2.0, 1.5, 2.0, 1.75, 1.75 mm, respectively. The plug flow velocity profiles are observed at the inlet of blood flow, whereas the anatomical difference between the arterial sides leads to an asymmetric distribution of the velocity profiles [36]. Flow patterns in blood vessels can be illustrated by the blood flow colored by the magnitude of velocity. The velocity waveform can be compared with the velocity contour plot at characteristic locations. Based on the generalized power law blood viscosity model, Fig. 3 (bottom) shows a representative data set for the velocity in the ITA artery [28].

3.2. Particle trajectory

Externally implanted magnets have been used to mimic the targeted delivery of the DAS-MNM drugs. A magnetic field can easily be manipulated to cover the desired location by orientation, and strength. First, the trajectory of the particles without any external magnetic field is examined. Particle distribution in arterial vessels can be seen in Fig. 4. Different colors correspond to different velocities of the particles. High-velocity particles are denoted by red, whereas low-velocity particles are denoted by blue. Low blood velocity near the lumen wall is lead to a slow particle movement within the lumen. A few particles remain near the endothelium layer because of low blood velocity in the boundary layer. But, the numerical analyses revealed that these effects do not remain constant because most particles leave the lumen after 1 s, while at least 10 s resident time is required to ensure MDT stimulation is effective [37].

Second, according to a number of studies, a magnet with a maximum magnetic field strength of 2 (T) is applied to deliver the target drug to ensure that the maximum exposure of the arterial magnetic field does not exceed 0.5 (T) [37].

Figure 5 shows the magnetic field and magnet geometry based on our numerical simulation. It can be seen that the magnetic field strength decreases rapidly as the distance from the magnet increases. The typical magnetic field strength at the target location was approximately 0.5 T. The magnetic field is applied 500 µm above the artery wall at the target site to obtain a magnetic flux density of 0.5 (T) within the artery.

The drug particles trapped by the external magnetic field at different times are depicted in Fig. 6. The MDT stimulation starts within the first 10 s of the resident time. The high-velocity particles of a wider range of DAS-MNM particle sizes were beginning to move at 5 s and collect near the source of the magnetic field at the arterial wall than in other positions. The particles continue to move towards the magnetic field and within 20 s, the capture efficiency of DAS-MNM reaches more than 90% (Fig. 6(d)). It is clearly noticed the presence of a region free of drug particles near the center of the artery model (especially in the time range t = 20 seconds), which indicates that the DAS-MNM particles are distributed at the entrance at successive times intervals. Also, it can be seen that the DAS-MNM particles accumulated near the external magnetic field source at the arterial wall while the other areas remained empty after 60 s confirming the enhanced deposition due to the imposed magnetic field.

3.3. Particle Capture
The released DAS-MNM particles into the artery are steered to the targeted site by an external magnet. The effect of magnetic field strength (MFS), magnet size, particle size, relative magnetic permeability of particles, and initial distribution of particles on MDT were studied. The results indicated that particle diameter and MFS are more influential on particle deposition rate. Figure 7 shows that the number of trapped particles increases with increasing both magnetic field strength and DAS-MNM particle size. Although, the magnetophoretic force and drag force have no linear relationship with the particle diameter (Equations (10) and (13)). For instance, the number of trapped particles increases substantially when particle size increases by one order of magnitude without changing the MFS.

Four different sizes of external permanent magnets are simulated to examine the effect of magnet size on MDT performance and the total number of trapped particles as shown in Fig. 8. With a larger magnet size, the tissue can be covered more widely, thus enhancing the chance of particles being retained at the targeted site. Even though the magnet size is effective in particle trapping, it is not linearly proportional to particle retention as the magnet size is increased. Thus, the most effective MDT performance can be achieved by selecting a proper magnet size.

The retention of particles at the tissue site is improved by increasing the magnetic permeability of the particles, as shown in Fig. 9. The results indicate that particle relative permeability in the range of 3 to 15 does not affect particle trapping very much, when the particle permeability increases from 3 to 15, increasing particle retention from almost 7–10% occurs, with particle diameters of 250 nm and 500 nm, respectively.

Moreover, three different sites of the initial particle distribution release on the particle retention were investigated. It is a uniform distribution at the entrance and the distribution depends on the speed and at the top of the entrance. Figure 10 shows the effect of the initial distribution of DAS-MNM on particle trapping. It is clearly notice the particle retention is greatly influenced by the particle release mechanism in the target tissue. Compared to the uniform or velocity-based particle release scenarios at the entrance, the particles ejecting close to the upper wall result in a high particle trapping rate.

### 3.4. Magnetic-based drug/cargo delivery

One of the most important MDT methods with high accuracy for effective target drug delivery is use the micro motors in a single drug/cargo. These motors have a different sizes and can be guided to their desired locations by applying an external magnetic field (e.g. 50 mm Janus micro motors) [38]. To investigate the feasibility of MDT method for artery drug/cargo delivery, various sizes and releasing locations of single DAS-MNM drugs/cargos throughout the ITA arteries are studied. A particle is trapped in the desired location in the artery wall when the magnitude of the magnetic force is greater than the blood drag force that transport the particles. Figures (11–13) show that a wider range of DAS-MNM particle diameters is trapped near the magnet wall than other positions. A higher retention probability was found near the magnet when the particles had a diameter of 500 mm in different initial positions. To achieve a successful and non-invasive drug delivery through the arteries, the particle size, magnetic field, and initial releasing location must be adjusted simultaneously.
4. Conclusions

This work highlights on the MDT performance and develops a comprehensive model to investigate the drug particle trajectories of DAS-MNM released in ITA blood flow by an external magnetic field for breast cancer therapy. The particle trajectory results confirmed the successful MDT using an external magnetic field with a capture efficiency of more than 90%, through the accumulation of a wide range of particle sizes of DAS-MNM and at the arterial wall near the externally magnetic field source than in other positions. Moreover, the particle retention increased with an increase in both MFS and particle diameter within the target tissue, while the particle permeability does not have a significant effect on the trapped particles. The drug/cargo delivery results show that the successful and non-invasive drug delivery through the arteries attaining when the particle size, magnetic field, and initial releasing location adjustable simultaneously.

Declarations

Ethics approval and consent to participate:

Informed consent was obtained from all individual participants included in the study.

Consent for publication:

The authors affirm that human research participants provided informed consent for publication.

Availability of data and materials

The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Competing interests

The authors have no relevant financial or non-financial interests to disclose.

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Author contributions

All authors contributed to the study conception and design. Data collection and analysis were performed and the first draft of the manuscript was written by [Saad Sulttan] and all authors commented on previous versions. All authors read and approved the final manuscript.

Conflict of Interest
The authors of this research acknowledge the originality of their research. This research has not been published before. It is not under consideration for publication elsewhere. The authors approved the submission of this article to the Drug Delivery and Translational Research.

References


Figures
Figure 1

Schematic depiction for the MDT model. (a) Internal thoracic artery (ITA) and its branches in the human body [26], (b) Schematic depiction of ITA for the MDT model.
Figure 2

The two-dimensional model mesh which is a representative for arterial flow. Domain (1) magnetic field, domain (2) external magnet and domain (3) is blood vessel of the ITA artery.
Figure 3

(Top) The physiological waveform used in this study was based on the work of Matsuo and co-workers [35]. (Bottom) The velocity magnitude in the simulated arterial flow corresponds to the velocity profile illustrated in top figure. The red arrows denote the direction of flow at the inlet.
Figure 4

Particle trajectory distribution without external magnetic field, the velocity magnitude of the particles are represented by the colour contour. (Particle size =500 nm).
**Figure 5**

Magnetic field strength and magnet geometry. The magnetization vectors are shown by the white arrows and the magnetic flux density is represented by the colour contour.

**Figure 6**

The effect of a permanent magnet on particles retention. The magnetization vectors are shown by the white arrows and the magnetic flux density and the velocity magnitude of the particles are represented by the colour contour. (Particle size =500 nm). (a) at t=10 s, (b) at t=20 s, (c) at t=60 s and (d) the capture efficiency of DAS-MNM.
Figure 7

The effects of magnetic field strength (MFS) and particle diameter on the efficacy of DAS-MNM particle trapping.
Figure 8

The effect of magnet size on the efficacy of DAS-MNM particles trapping, MFS=2T.

Figure 9

The effect of particles magnetic permeability on DAS-MNM particle retention, MFS=2T.
Figure 10

The effect of the initial distribution of DAS-MNM on particle trapping
Figure 11

Single particle position (x, y) moving through the artery with different diameters and released near the upper wall in the presence of external magnetic field.
Figure 12

Single particle position (x, y) moving through the artery with different diameters and released at the middle of the artery in the presence of external magnetic field.
Figure 13

Single-particle position \((x, y)\) moving through the artery with different diameters and released near the lower wall in the presence of external magnetic field.

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