

Particle-based Magnetohydrodynamics Modeling and Visualization: Part I - Theoretical Model

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ABSTRACT. In this paper a theoretical particle-base model for modeling of the magnetohydrodynamics (MHD) phenomena is presented. The fluid is modeled as a three dimensional particles system. The Navier-Stokes equation, containing the surface tension term formulation, are discretized using moving particles and their interaction models. Each particle moves accordingly with its own mass and the external/internal forces applied on it. The forces are evaluated on each particle. The purpose of this approach is to emphasize that this method allows a good way for the study and design of the MHD process.

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1. Introduction

Modeling techniques are indispensable tools for the analysis of dynamical systems such as computational fluid dynamics (CFD) or MHD. The modeling of the inside phenomena in dynamical systems is a challenging subject not only from an analytical or numerical point of view, but how to get insight to their dynamical behavior and have a better understanding of the complex flow phenomena.

The importance of fluid flow phenomena in CFD or MHD (magnetic stirring or electromagnetic levitation) has long been recognized. An analytically study for the fluid dynamical aspects of the MHD process for a levitated cylinder has been considered in [22]. The fluid flow computation and visualization using a finite difference scheme coupled with the electromagnetic forces derived analytically have been studied in [16]. Other theoretical approaches for flow modeling in MHD can be found in [1, 2, 3, 5, 6, 7].

For the modeling of the fluid flow phenomena two main categories of methods are used: Lagrangian formulation, a method that discretize the fluid using particles and Eulerian formulation, a method that discretize the problem using a subdivision of the spatial domain and control fluid flow in each cell.

A Smoothed particle hydrodynamics (SPH) formulation, with the space non-uniformly sampled using particles, was developed in [11, 15] using a Lagrangian formulation. A molecular dynamics technique was used in [17] to describe particle interactions, for simulations of melting materials and viscous fluids.

In [8] the SPH concepts were applied for the simulation of highly deformable bodies. Using a SPH particle-based method [18, 19], a 3D simulation for material properties ranging from highly plastic to stiff elastic was implemented.

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A spring-particles model for melting solids with various forces applied to their neighbors was developed in [23]. A similar model using springs was developed in [9].

The work in the present paper is dedicated to describe a theoretical model for modeling of MHD phenomena using particles with the specific goal of analyzing the fluid interface and flow visualization.

The fluid is modeled as a three dimensional particles system using the Moving-Particle Semi-implicit (MPS) method [12, 21]. In this mesh-free method the interaction between particles is specified by a weight function which relates a particle with others in its vicinity. MPS method has been proved suitable in dealing with large deformations interface [20, 24].

To describe the fluid motion the Navier-Stokes equation containing the surface tension term formulation has been used. The Navier-Stokes equation has been solved using a Lagrangian formulation, the moving particles and their interaction models (representing gradient, laplacian and divergence) of the MPS method. Comparing with other application based on the Eulerian formulation, the Lagrangian modeling allow an easy perception of flow data. The boundary conditions has been imposed and a surface tension model [4] (continuum surface force (CSF) model) of the particles that lie on the surface has been presented.

The external/internal force [9] (gravitational force, electromagnetic force, forces between particles) formulation in Navier-Stokes equation, evaluated on each particle, and the associated boundary conditions, for the case of electromagnetic levitation (levitated droplet) and electromagnetic stirring (rotating cylindrical sample) are presented.

2. Governing Equations

Governing equations to describe fluid flows in the CFD or MHD process are the continuity equation, written in a general form as

$$\frac{D\rho}{Dt} = -\rho(\nabla \cdot \mathbf{u}) = 0, \quad (1)$$

and the momentum equation *containing the surface tension* term

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \eta\nabla^2\mathbf{u} + \rho\mathbf{g} + \mathbf{F} + \sigma k\delta\mathbf{n}, \quad (2)$$

where $\frac{D\mathbf{u}}{Dt} = \frac{\partial}{\partial t} + (\mathbf{u} \cdot \nabla)$, t is the time, \mathbf{F} is the force density exerted on the fluid, k is the mean curvature of the interface, δ is the Dirac delta function that is zero everywhere except at the interface, \mathbf{n} is the unit normal vector to the interface, σ is the surface tension coefficient and $\sigma k\delta\mathbf{n}$ represent the surface force per unit interfacial area.

Instead of a surface tensile force or surface pressure boundary condition applied at a discontinuity, surface tension is calculated by applying at extra body force in the momentum equation (Eq.(2)). Using the continuum surface force (CSF) model [4], surface tension is modeled as a volume force acting on the fluid interfaces (particles that are regarded as the interface). Surface tension modeled with the continuum method eliminates the need for interface reconstruction and simplifies the calculation of the interface [13], enables accurate modeling of three dimensional flows and does not impose any modeling restrictions on the dynamic evolution of fluid interfaces having surface tension.

3. Particle Interaction and Surface Tension Model

3.1. Mathematical Model of MPS-method. Using the work of [12, 13, 21, 24], all the terms expressed by differential operators in the momentum equation will be replaced by particles interactions. For this, the continuous media is modeled as a three dimensional particles system, a particle model normally distributed in its initial configuration.

To discretize the continuous media, it is considered that a particle i interacts with its neighboring particles j according to a weight function $w(r)$, defined as

$$w(r) = \begin{cases} \frac{r_e}{r} - 1 & \text{if } 0 \leq r < r_e \\ 0 & \text{if } r_e \leq r \end{cases}, \quad (3)$$

where $r = |\mathbf{r}_j - \mathbf{r}_i|$ is the distance between the particles i and j and r_e represents the radius of the interaction (Fig. 1.a). An example of weight function is given in Fig. 1.b.

The particle number density at coordinate \mathbf{r}_i is defined as

$$\langle n \rangle_i = \sum_{j \neq i} w(|\mathbf{r}_j - \mathbf{r}_i|), \quad (4)$$

where $j \neq i$ means that the contribution from particle i to itself is not considered. For simplicity, it is considered that the particles have the same mass m . The, the fluid density is proportional to the particle number density $\langle \rho \rangle_i = m \frac{\langle n \rangle_i}{\int w(r) dv}$.

A gradient vector is defined by $(\phi_j - \phi_i)(\mathbf{r}_j - \mathbf{r}_i) / |\mathbf{r}_j - \mathbf{r}_i|^2$, where ϕ_i and ϕ_j are scalar quantities and \mathbf{r}_i and \mathbf{r}_j represent particles co-ordinates. The gradient vector at particle i can be expressed as

$$\langle \nabla \phi \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \left[\frac{(\phi_j - \phi_i)}{|\mathbf{r}_j - \mathbf{r}_i|^2} (\mathbf{r}_j - \mathbf{r}_i) w(|\mathbf{r}_j - \mathbf{r}_i|) \right], \quad (5)$$

where d is the number of space dimensions and n^0 is the particle number density in the initial configuration.

The divergence operator can be modeled in the same way as the gradient vector (Fig. 1.a). The velocity divergence between two particles i and j is defined by $(\mathbf{u}_j - \mathbf{u}_i) \cdot (\mathbf{r}_j - \mathbf{r}_i) / |\mathbf{r}_j - \mathbf{r}_i|^2$ and the velocity divergence at the particle i is given by

$$\langle \nabla \cdot \mathbf{u} \rangle_i = \frac{d}{n^0} \sum_{j \neq i} \left[\frac{(\mathbf{u}_j - \mathbf{u}_i)}{|\mathbf{r}_j - \mathbf{r}_i|^2} (\mathbf{r}_j - \mathbf{r}_i) w(|\mathbf{r}_j - \mathbf{r}_i|) \right]. \quad (6)$$

The Laplacian operator can be interpreted as if a fraction of a scalar quantity at particle i is dispersed to a particle j according to the weight function, and can be written as

$$\langle \nabla^2 \phi \rangle_i = \frac{2d}{\lambda n^0} \sum_{j \neq i} [(\phi_j - \phi_i) w(|\mathbf{r}_j - \mathbf{r}_i|)], \quad (7)$$

where λ can be approximated as $\lambda = \frac{\sum_{j \neq i} [|\mathbf{r}_j - \mathbf{r}_i|^2 w(|\mathbf{r}_j - \mathbf{r}_i|)]}{\sum_{j \neq i} [w(|\mathbf{r}_j - \mathbf{r}_i|)]}$.

Using Eqs.(1) and (2) a Poisson equation for the pressure is obtained

$$\langle \nabla^2 p^{n+1} \rangle_i = \frac{\rho}{\Delta t} \langle \nabla \cdot \mathbf{u}^* \rangle. \quad (8)$$

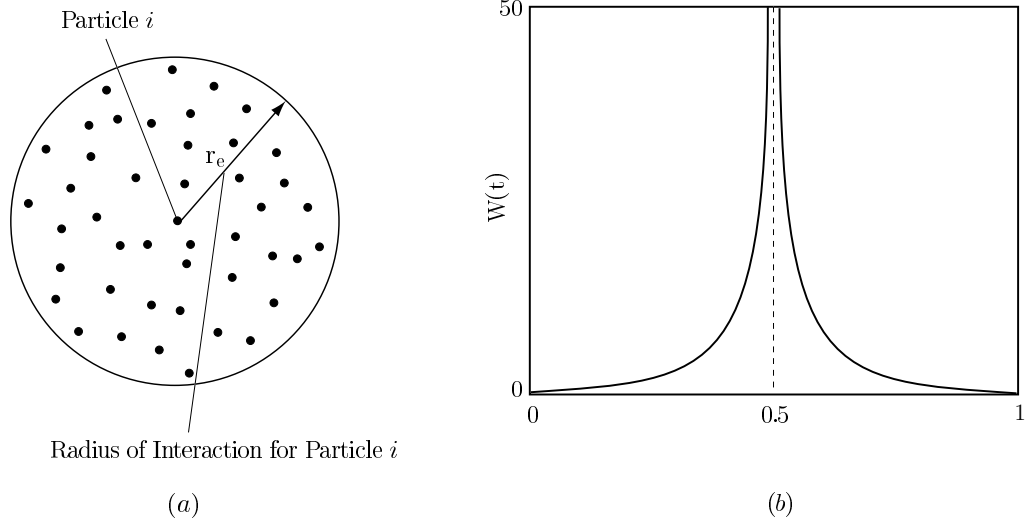


FIGURE 1. (a) Radius of Interaction, and, (b) An Example of a Weight Function

The left side of Eq.(8) is the Laplacian model and can be calculated using Eq.(7), the right side of Eq.(8), is the velocity divergence, and can be calculated using Eq.(6).

The temporal velocity can be calculated using

$$\frac{\mathbf{u}_i^{**} - \mathbf{u}_i^*}{\Delta t} = -\frac{\Delta t}{\rho} \langle \nabla P^{n+1} \rangle, \quad (9)$$

where \mathbf{u}_i^* is the temporal velocity explicitly calculated, \mathbf{u}_i^{**} is the new time velocity and Δt is the time increment. The right side of Eq.(9) is the gradient model and can be calculated using Eq.(5). After pressure calculation, the new time velocity \mathbf{u}_i^{**} can be calculated using Eq.(9).

3.2. Surface Tension Model. Surface tension is computed on the fluid interface. A surface tension model [20] is extended to a three dimensional computation. A new particle number density of the particles that lie on interface is considered to be

$$n_i^{st} = \sum_{j \neq i} w^{st} (|\mathbf{r}_j - \mathbf{r}_i|),$$

where the new weight function is

$$w^{st}(r) = \begin{cases} 1 & \text{if } 0 \leq r < r_e^{st} \\ 0 & \text{if } r_e^{st} \leq r \end{cases}.$$

Because the particle number density can increase near the interior of the droplet, and this can lead to errors in the calculation of curvature, a new particle number density for the particles that lies on the interface is calculated

$$n_i^{st_new} = \sum_{j \neq i} w^{st_new} (|\mathbf{r}_j - \mathbf{r}_i|),$$

where another weight function

$$w^{st_new}(r) = \begin{cases} 1 & \text{if } 0 \leq r \leq r_e^{st} \text{ and } n_j^{st} > n_i^{st} \\ 0 & \text{if otherwise} \end{cases},$$

is used.

The unit normal vector \mathbf{n} vertical to the interface and the curvature k on the fluid interface are calculated using the w^{st} weight function and the particle number density. The particle number density for six different positions around the particle i can be expressed by $n_i^x(\mathbf{r}_i + d_{st}\mathbf{n}_x)$, $n_i^{-x}(\mathbf{r}_i - d_{st}\mathbf{n}_x)$, $n_i^y(\mathbf{r}_i + d_{st}\mathbf{n}_y)$, $n_i^{-y}(\mathbf{r}_i - d_{st}\mathbf{n}_y)$, and $n_i^z(\mathbf{r}_i + d_{st}\mathbf{n}_z)$, $n_i^{-z}(\mathbf{r}_i - d_{st}\mathbf{n}_z)$. The unit normal vector at particle i that lies on the interface is computed as

$$\mathbf{n}_i = \frac{\mathbf{s}_i}{|\mathbf{s}_i|},$$

where $\mathbf{s}_i = \frac{n_i^x - n_i^{-x}}{2l_0}\mathbf{n}_x + \frac{n_i^y - n_i^{-y}}{2l_0}\mathbf{n}_y + \frac{n_i^z - n_i^{-z}}{2l_0}\mathbf{n}_z$, and \mathbf{n}_x , \mathbf{n}_y , \mathbf{n}_z are the unit normal vectors in the x , y and z directions.

The curvature of the interface is computed as

$$k = \frac{1}{R} = \frac{2 \cos \theta}{r_e^{st}},$$

where $R = \frac{r_e^{st}}{2 \cos \theta}$ represent the curvature radius, r_e^{st} represents the radius of the interaction for surface tension and $\theta = \frac{\pi n_i^{st, new}}{2 n_i^{st}}$.

4. Electromagnetic Forces and Boundary Conditions

4.1. Electromagnetic levitation. The levitation system shown in Fig. 2.a is composed of N ($N = 6$) coaxial circular loops of current lying in parallel planes. The radius of each loop is denoted by b_k , $k = 1, 2, \dots, N$. For the general case, each loop carry an alternating electric current $\Re[I_k e^{j\omega t}]$, where I_k is the peak value, ω is the angular frequency of the imposed field ($\omega = 2\pi f$, where f is the frequency), t is the time, $j = \sqrt{-1}$ and $\Re(\cdot)$ denotes the real part of the complex current. The body to be levitated is a conductive droplet of radius R , mass M , electric conductivity σ_c , and magnetic permeability μ .

The unit vector of the Cartesian reference frame (x, y, z) are denoted by \mathbf{i} , \mathbf{j} and \mathbf{k} and the unit vectors of the spherical reference frame (r, θ, φ) by \mathbf{e}_r , \mathbf{e}_θ and \mathbf{e}_φ . The k^{th} loop is defined by r_k and α_k , where r_k is the length from the origin to the k^{th} loop and α_k is the solid angle subtended by the k^{th} loop with respect to the spherical reference frame as shown in Fig. 2.a.

The corresponding 3D particle system model of the levitated sample is shown in Fig. 2.b.

The electrodynamic and hydrodynamic phenomena occurring in the magnetic levitation process can be described by a set of the following coupled Maxwell equations

$$\nabla \cdot \mathbf{D} = \mathbf{u}, \quad \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = \mathbf{0}, \quad \nabla \cdot \mathbf{B} = \mathbf{0}, \quad \nabla \times \mathbf{H} = \mathbf{J},$$

along with Eqs.(1) and (2) i.e., continuity equation and momentum equation, and with the constitutive relationship linking the current density with other field variables, i.e. Ohm's law written for a moving medium

$$\mathbf{J} = \sigma_c (\mathbf{E} + \mathbf{u} \times \mathbf{B}).$$

In the above equations \mathbf{J} is the induced eddy current density, \mathbf{H} is the magnetic flux density, \mathbf{D} is the electric displacement, \mathbf{B} is the magnetic field, \mathbf{E} is the electric field, \mathbf{F} is the Lorentz force density, \mathbf{u} is the velocity field, ρ is the density, p is the pressure,

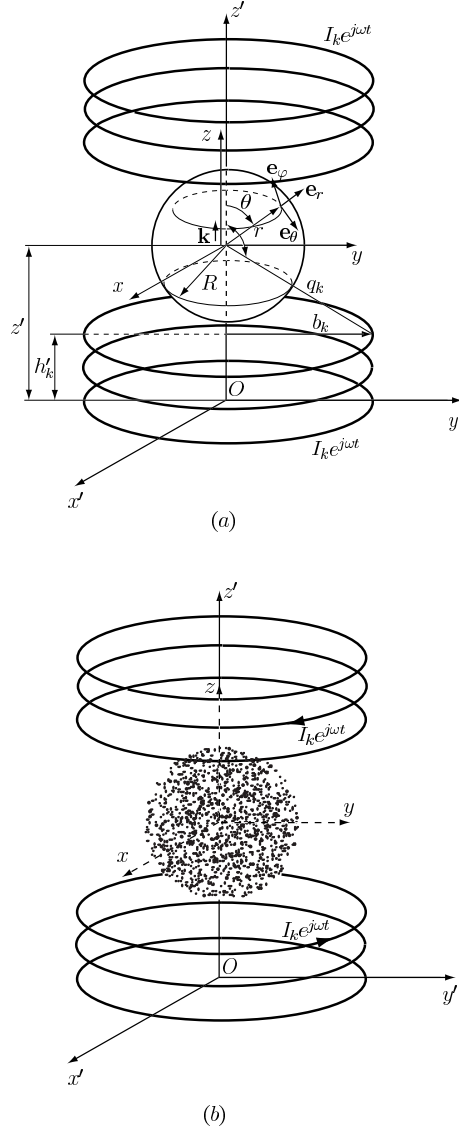


FIGURE 2. (a) Levitation System - Coil and Levitated Droplet, and, (b) Particle Model of the Levitated Droplet

η the viscosity of the fluid, \mathbf{g} the gravity and t is the time. The local distribution of the electromagnetic force fields serves as a starting point for both the fluid flow calculation and the global levitability of the system. The time-averaged Lorentz force density exerted on a levitated sphere is given by

$$\mathbf{F} = \frac{1}{2} \Re(\mathbf{J} \times \mathbf{B}^*), \quad (10)$$

where $\Re(\cdot)$ and $*$ are the real part and the complex conjugate of a complex variable, respectively.

Using the work of [14], the values of r and θ components of the time averaged Lorentz Force for a single current loop (k -loop) can be calculated using

$$\begin{aligned}
 F_r &= -\frac{\omega\sigma_c\mu^2 I^2 \sin^2 \alpha_k}{8r} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{2m+1}{m(m+1)} \frac{2n+1}{n(n+1)} \left(\frac{R}{r_k}\right)^{m+n} \\
 &\quad \times P_m^1(\cos \alpha_k) P_m^1(\cos \theta) P_n^1(\cos \alpha_k) P_n^1(\cos \theta) \\
 &\quad \times \Re \left[\frac{j I_{m+1/2}(k_p r)}{I_{m+1/2}(k_p R) I_{n-1/2}(k_p^* R)} \left(\frac{I_{n-1/2}(k_p^* r)}{k_p R} - \frac{n I_{m+1/2}(k_p^* r)}{r R \omega \sigma \mu} \right) \right], \\
 F_\theta &= \frac{\mu (I \sin \alpha_k)^2}{8r^2 R} \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{(2m-1)(2n-1)}{m(m+1)} \left(\frac{R}{r_k}\right)^{m+n} \\
 &\quad \times \Re \left[\frac{j I_{m+1/2}(k_p r) I_{n-1/2}(k_p^* r)}{I_{m-1/2}(k_p R) I_{n-1/2}(k_p^* R)} \right] \\
 &\quad \times P_m^1(\cos \alpha_k) P_m^1(\cos \theta) P_n^1(\cos \alpha_k) P_n^1(\cos \theta), \tag{11}
 \end{aligned}$$

where $P_n^1(\cos \theta)$ are the associate Legendre polynomials or the Legendre function of the first kind of order n , $I_{n+1/2}$ are the modified Bessel functions of the first kind of order $n+1/2$, k_p is a system parameter, $k_p = j\omega\mu\sigma$, k_p^* is the conjugate of k_p , ω is the angular frequency of the imposed field ($\omega = 2\pi f$, where f is the frequency), t is the time, $j = \sqrt{-1}$ and $\Re(\cdot)$ denotes the real part of the complex current. The body to be levitated is a conductive droplet of radius R , mass M , electric conductivity σ_c , and magnetic permeability μ .

In order to implement the boundary conditions on the fluid interface, the Laplacian model defined as in Eq.(7) is used. The Neumann boundary condition applied to the pressure calculation via Poisson equation is imposed. The Neumann condition states that the pressure change along the normal must be zero. The Neumann boundary conditions specify the normal component at the boundaries, and for this case, that the pressure calculated at each particle on the boundary is equals with the outside pressure. So, the Neumann boundary condition is satisfied if the pressure of a particle i on the boundary is equal with the outside pressure. Supposing that the pressure of a particle j outside the boundary is p_j , the Neumann boundary condition may be approximated using the next alternative expression of Eq.(7)

$$\langle \nabla^2 p \rangle_i = \frac{2d}{\lambda n^0} \sum_{j \neq i \text{ and } j \neq \text{out}} [(p_j - p_i) w(|\mathbf{r}_j - \mathbf{r}_i|)].$$

4.2. Electromagnetic stirring. Electromagnetic stirring is now a well technique in continuous casting of round strands. The method is usually based on the phenomena that when a sample of viscous liquid metal confined to a cylindrical crucible, rotates in an applied magnetic field, and in the presence of gravity, circulating eddy currents are induced and a Lorentz force is produced. For the present case, the transverse magnetic field imposed upon the rotating melt is assumed to be stationary and uniform. In addition to the applied magnetic field, there is an induced magnetic field produced by an electric current in the conducting fluid. To simplify the computation of the flow and force fields, the melt is considered to be electrically and thermally conducting and incompressible. The rotating cylindrical sample is shown in Fig. 3.a, and the 3D particles system model in Fig. 3.b.

The equations governing the time-dependent incompressible viscous flow in the crucible, including electrodynamic effect, are the stationary Navier-Stokes equation

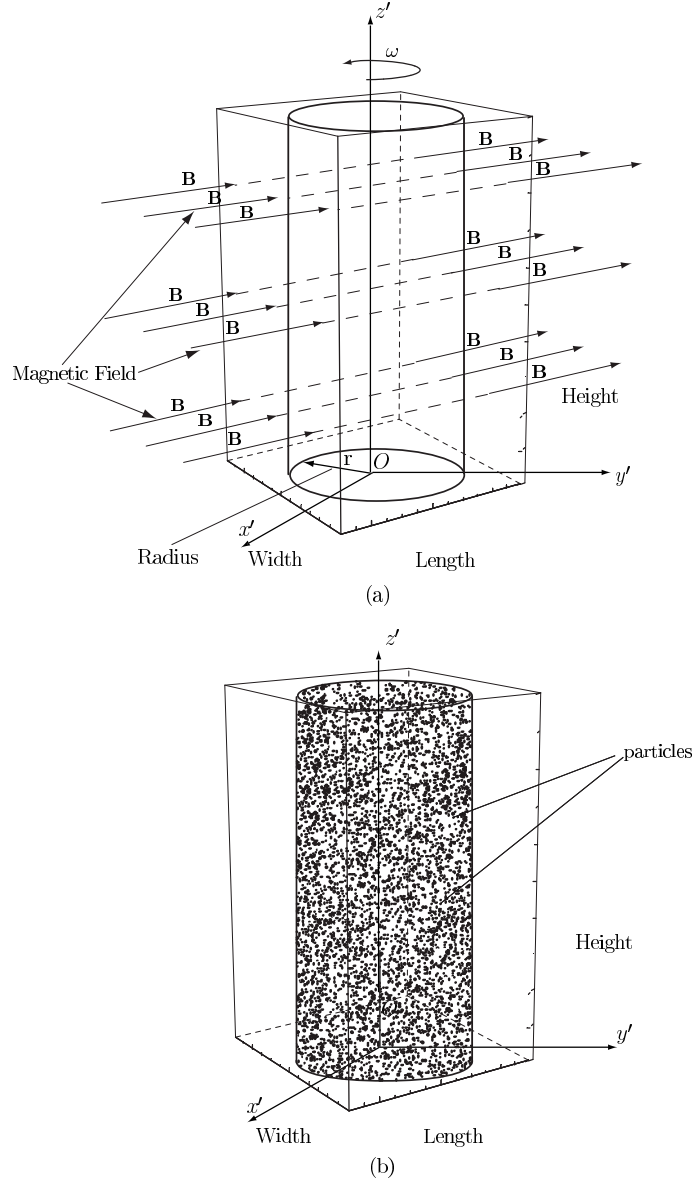


FIGURE 3. (a) Magnetic Stirring System - Rotating Cylindrical Sample, and, (b) 3D Particle Model of the Sample

with Boussinesq approximation, along with the the continuity equation. Equations (1) and (2) must be supplement with a boundary condition for the fluid velocity at the wall, and equation (2) with the Boussinesq approximation.

According to Maxwell equations and Ohm's law, the Lorentz force can be computed using

$$\mathbf{F} = \mathbf{J} \times \mathbf{B}, \quad (12)$$

where \mathbf{J} is the current density and \mathbf{B} is the magnetic field.

The body force \mathbf{F} at the right side of Eq.(2) (electromagnetic stirring case), will include the gravity, buoyancy and the Lorentz forces. A Boussinesq approximation is used to account for buoyancy forces due to temperature gradients, that is, that the temperature T fluctuates in a narrow range about a reference temperature T_{ref} , and the density, in this temperature range, decreases linearly with T ,

$$\frac{\rho}{\rho_{ref}} = 1 - \beta(T - T_{ref}) \quad (13)$$

where ρ and β denote the density and thermal expansion coefficient of the fluid at the reference temperature. The force of gravity is given by

$$\rho g = \rho_{ref} g - \beta \rho_{ref} (T - T_{ref}) g. \quad (14)$$

where $\beta \rho_{ref} (T - T_{ref}) g$ represents the buoyancy force.

The Lorentz force term will be different for transverse or vertical, stationary or alternating magnetic fields. For Lorentz force computation, a cylindrical coordinate system (r, θ, z) with the attached unit vectors $\mathbf{s}_r, \mathbf{s}_\theta, \mathbf{s}_z$, and with the z axis along the cylinder vertical axis is used. In the case of transverse stationary and uniform magnetic field $B_0 = B_0(I_r \cos \theta - I_\theta \sin \theta)$, the components for the Lorentz force (for more details see [10]) can be written as,

$$\begin{aligned} F_r &= -\sigma B_0 [\phi_z \sin(\theta) + B_0 u \sin^2(\theta) + \frac{1}{2} B_0 v \sin(2\theta)], \\ F_\theta &= -\sigma B_0 [\phi_z \cos(\theta) + \frac{1}{2} B_0 u \sin(2\theta) + B_0 v \cos^2(\theta)], \\ F_z &= -\sigma B_0 [\phi_z \sin(\theta) + \frac{1}{r} \phi_\theta \cos(\theta) - B_0 w], \end{aligned} \quad (15)$$

where ϕ denotes the electric potential, ϕ_z denotes the z component of the electric potential, u, v and w are the radial, tangential and vertical velocity components, respectively. The tangential component of the Lorentz force is in a direction opposite to the fluid rotation, and the radial component is in the direction related to the position coordinates (r, θ) . The tangential component of the Lorentz force can be evaluated as $F_t = \frac{1}{2} \sigma \omega r_0 B_0^2 \sin(2\theta)$. For the cylinder, all variables except θ are independent of z .

For the constant temperature boundary condition, the heat flux across the walls is considered to be constant. It is determined by considering the temperature of the computing point near the source and heat flux,

$$T_{ref}^{n+1} = \frac{1}{n_i} \sum_j \left[T_j^{n+1} - \frac{q''}{k} \Delta y_j \right] w(|\mathbf{r}_j - \mathbf{r}_i|), \quad (16)$$

where k is the thermal conductivity and q'' is the flux.

5. Conclusions

In this work, the modeling of the magnetohydrodynamic phenomena related to electromagnetic levitation (EML) and magnetic stirring, has been considered. The fluid was modeled as a three dimensional particles system. The MPS method which is based on moving particles and their interaction has been described. Grids commonly used in FEM-based and Eulerian approaches are not necessary. The partial differential equations, i.e. Navier-Stokes equations, are discretized by particle interaction models

according to a weight function. A surface tension term formulation in the Navier-Stokes equation was used. A calculation model of surface tension was presented.

Two particular models have been taken into consideration: levitated droplet for the EML case and a rotating cylindrical sample for the electromagnetic stirring. The external/internal force have been evaluated on each particle, and the associated boundary conditions imposed.

Using this approach it will be show through numerical simulation that this method allows a good way for the study of fluid flows time-dependent phenomena i.e. three-dimensional unsteady flows, complex turbulent flows, and associated surface deformation.

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