Numerical Simulation of Magnetic Fields and Spin Velocity for Unsaturated Ferrofluid Driven by External Static and Rotating Magnetic Fields

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Introduction

Superparamagnetic iron oxide (SPIO) agents are potent MRI contrast agents [1]. Included in this category of contrast agents is ferrofluid, which consists of magnetite (Fe_3O_4) nanoparticles in a liquid suspension. Field inhomogeneity experienced by water interacting with one or more magnetite particles is well understood [2] and theoretical predictions for T1 and T2 match experimental results [3]. This work investigates ferrofluids in the non-saturated regime, where the magnetic moment of the ferrofluid is coupled to the local magnetic field by the ferrofluid susceptibility. For ferrofluid in a low-strength DC field, the susceptibility is approximately a constant, χ_0. In a rotating magnetic field, the susceptibility is a 3x3 complex tensor expression dependent upon the ferrofluid characteristic time constant, τ, the rotating magnetic field frequency, Ω, the ferrofluid's DC susceptibility, χ_0, and the ferrofluid spin velocity vector, $\boldsymbol{\omega} = \omega_z \bar{i}_z$ [4], [5]. Numerical simulations of a rotating magnetic field in the $\{xy\}$ plane are employed to demonstrate the effect of these parameters on the magnetic field in water in the macroscopic vicinity of a compartment of ferrofluid.

Methods

To investigate the effect of rotating transverse magnetic fields in the presence of unsaturated ferrofluid, *Comsol Multiphysics* (*Comsol AB*, Stockholm), a FEA solver, was used to simulate the field distribution in two concentric cylinders filled with ferrofluid (center), and water (Fig.1), both assumed infinitely long in z such that the fields in the z and $\{xy\}$ domains are uncoupled. The decoupling is shown from the solution (Eq. 4) to Shliomis' First Ferromagnetic Relaxation Equation [5] (Eq.1) with zero flow velocity, in terms of complex field amplitudes (Eq.2), in sinusoidal steady state for an unsaturated ferrofluid in the linear regime under rotating magnetic field excitation in the $\{xy\}$ plane, at electrical frequency, Ω. This analysis examines the field solutions for a cross-sectional slice in the $\{xy\}$ plane, ignoring effects due to the cylinder ends. The complex field amplitudes employed for ferrofluid magnetization vector, **M**, and magnetic field intensity, **H,** are related to their corresponding time domain equivalents by Eq. 2, where $\bar{i}_x$, $\bar{i}_y$ and $\bar{i}_z$ are unit vectors along the Cartesian axes. The ferrofluid spin velocity (Eq. 3) is then $\boldsymbol{\omega} = \omega_z \bar{i}_z$ where its expression follows from the conservation of angular momentum. The * notation denotes a complex conjugate and ζ is the ferrofluid vortex viscosity with units of Pascal-sceonds.

$$\partial \mathbf{M}/\partial t - \omega \times \mathbf{M} + (\mathbf{M} - \chi_0 \mathbf{H})/\tau = 0 \quad ...(1)$$

$$\mathbf{H} = \Re e\{\hat{\mathbf{H}}\, e^{j\Omega t}\},\ \hat{\mathbf{H}} = \hat{H}_x \bar{i}_x + \hat{H}_y \bar{i}_y + \hat{H}_z \bar{i}_z \quad ...(2a)$$

$$\mathbf{M} = \Re e\{\hat{\mathbf{M}}\, e^{j\Omega t}\},\ \hat{\mathbf{M}} = \hat{M}_x \bar{i}_x + \hat{M}_y \bar{i}_y + \hat{M}_z \bar{i}_z \quad ...(2b)$$

$$\omega = 1/(4\zeta)\Re e\{\mu_0 \hat{\mathbf{M}} \times \hat{\mathbf{H}}^*\} \quad ...(3)$$

$$\begin{pmatrix} \hat{M}_x \\ \hat{M}_y \\ \hat{M}_z \end{pmatrix} = \frac{\chi_0}{(1+j\Omega\tau)^2 + (\omega_z\tau)^2} \begin{pmatrix} 1+j\Omega\tau & -\omega_z\tau & 0 \\ -\omega_z\tau & 1+j\Omega\tau & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \hat{H}_x \\ \hat{H}_y \\ \hat{H}_z \end{pmatrix} \quad ...(4)$$

The ferrofluid characteristic time constant, τ, is dominated by either Néel or Brownian relaxation depending on the particle radius [4]. With careful selection of boundary conditions and an iterative solving approach, *Comsol* provides converged solutions of all relevant electromagnetic fields as well as the ferrofluid spin velocity, ω_z with a total computation time of approximately 10 minutes on a desktop PC.

Results

The solutions for concentrations of ferrofluid of 2.75% by volume of magnetite in water were found. The magnitude of the transverse magnetic field is plotted in Fig. 1 at time, t=0. The transverse field is normalized with respect to longitudinal magnetic field intensity in the water, H_0, where $B_0 = \mu_0 H_0$. B_0 is 0.5 T, the clockwise rotating magnetic field amplitude is 5% of B_0, the ferrofluid time constant, τ, is 10^{-8} s (corresponding to an approximate diameter of 5 nm for each particle in the ferrofluid) and $\Omega\tau = 1$. The transverse magnetic field is found to vary with position, as shown in the $\{xy\}$ cross-sectional slice in Fig. 1, but also with ferrofluid spin velocity, ω_z. As shown in Fig. 2, the variation of ferrofluid spin velocity, ω_z, with respect to $\Omega\tau$ is a maximum when $\Omega\tau = 1$ and increases with the ferrofluid time constant, τ. Selecting $\Omega\tau = 1$ maximizes the coupling terms in the solution to Shliomis' Relaxation Equation and, hence, results in the largest spin velocity in the ferrofluid.

Conclusions

Applying rotating magnetic field excitation in the $\{xy\}$ plane to an unsaturated ferrofluid results in a non-zero spin velocity for the nanoparticles. The angle deviation of the dipole field maxima away from the direction of the applied transverse rotating field (which is along the x axis at t=0) is due to both the ferrofluid time constant, τ, which acts to increase this angle deviation away from the rotating field, and the spin velocity, ω_z, which acts to decrease the angle deviation and move the dipole maxima into closer alignment with the applied rotating field.

References

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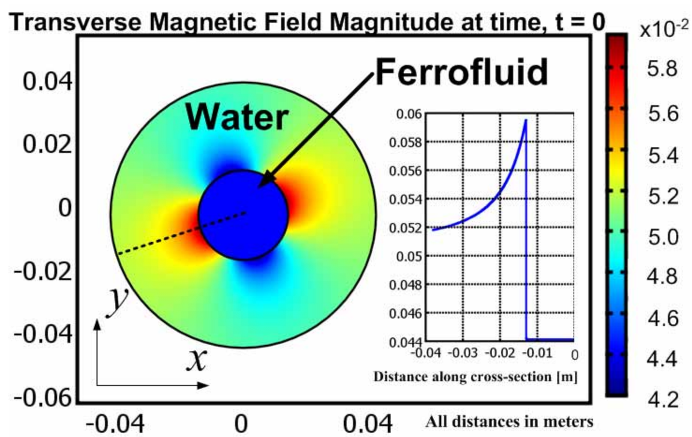

Fig. 1. Normalized transverse magnetic field intensity for 2.75% concentration ferrofluid in a 0.5 T $B_0\bar{i}_z$ field with 25 mT (5% of B_0) rotating magnetic field amplitude in the $\{xy\}$ plane. $\Omega\tau = 1$ and τ is 10^{-8} seconds.

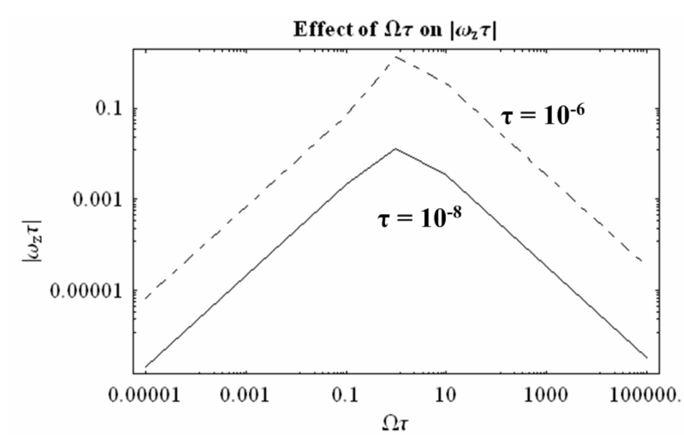

Fig. 2. The value of normalized spin velocity, $|\omega_z\tau|$, peaks when the normalized applied rotating field frequency, $\Omega\tau$, equals 1. Normalized spin velocity also increases with τ , and hence, also with magnetite nanoparticle radius.