TWO DIMENSIONS SIMULATION OF A MAGNETOTACTIC BACTERIA CELL EXPOSED TO AN ELECTROMAGNETIC FIELD AT 3 GHz

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Abstract: *The effect of the presence of magnetite nanoparticles inside biological objects when they are exposed to microwaves has not yet been investigated completely. Microwaves magnetic hyperthermia is a field under development, and the use of biogenic magnetite is a relatively new vista. In this regard, the present approach presents a first step in a modeling-simulation process focused on the computation of the absorbed power distribution in bacteria cells containing native magnetite nanoparticles in the form of chains (magnetosomes). The presented simulations' results refer to the simplest case of two-dimensional computation, which doesn't take into consideration the geometric and magnetic anisotropy characteristics of the real magnetosomes.*

Keywords: magnetosomes, magnetotactic bacteria, finite element simulation, magnetic hyperthermia, electromagnetics

1. Introduction

Magnetotactic bacteria represent a category of organisms that naturally produce and contain magnetic nanoparticles known as magnetosomes. The role and the benefits of these nanoparticles can be described in two directions. Firstly, they act as a compass aligning the bacteria with the magnetic field lines of the Earth's magnetic field, guiding it to an optimal place to live, mainly where the oxygen concentration is low, or even in anaerobic environments. Secondly, the tiny magnetic nanoparticles extracted from the bacteria prove their utility in two crucial, actual and in continuous development domains: medicine (in medical treatments' field based on electromagnetic stimulation of specific parts of the body previously "filled" with magnetite nanoparticles) and informatics (in the hardware production of the storage data devices) [1] – [3].

The bacteria produce magnetic nanoparticles by taking the iron from their surrounding environment and then transporting it to individual compartments called magnetosomes. Inside each of them, a small, near-perfect crystal of magnetite, a type of iron oxide (Fe_3O_4), grows. Practically, the magnetosome is a nanocrystal of magnetite enveloped in a thin biological membrane. A chain of magnetosomes is natively present in each magnetotactic bacteria cell (Fig. 1). It is worth mentioning that magnetosomes are very similar to the magnetic nanoparticles existing in the human brain [4].

The impact of ultra-high frequency range on magnetite nanocrystals has scarcely been investigated until now, mainly because very few researchers performed measurements of the magnetic properties of such crystals in the GHz frequency domain, with a few

exceptions [5] - [7]. Some absorption peaks appear in magnetic liquids containing magnetite nanoparticles and could have some interesting applications in the microwave region [8].

Therefore, this paper aimed to perform a set of simulations in Comsol Multiphysics software in order to outline the dissipation/heating effect of exposure of a magnetotactic bacteria cell to a continuous wave of 3 GHz at a reduced field strength. Since previous simulations of magnetic nanoparticles heating due to microwave exposure are rare [9], [10], we have proposed here extraction of just some preliminary observations based on a set of simplified computations made on a model cell created in two dimensions.

Figure 1: Scanning-transmission electron microscopy of a Magnetospirillum gryphiswaldense cell and magnification of the inner magnetosome chain (courtesy of Dr. biol. Lucian Barbu-Tudoran from Babes-Bolyai University and INCDTIM in Cluj-Napoca, RO)

2. Simulations of the absorbed electromagnetic power in the bacteria cell and in the magnetosomes

The analysed cases describe the interaction of an incident electromagnetic plane wave penetrating from air to water (in which the cell is suspended) with an incident electric (E)-field strength in air of 10 V/m, directed on Oy direction (xOy will be the classical use of the space coordinates). The deposited power was 5 W at the working frequency of 3 GHz.

Figure 2: Overall design with bacteria cell, its interior magnetite crystals chain, and water's environment: dimensions [nm]

Figure 3: Magnetosome's dimensions [nm]

Four situations of wave's propagation were considered: a) the sample material is pure water; b) the sample contains water in which a bacteria cell is present; c) the sample is the same as in b)-case but inside the cell, a chain of magnetosomes exists; d) the sample is as in b)-case but in the cell, a cluster of magnetosomes exists.

The modeled geometry for all the simulations and the dimensions set for the water surface,

the bacterium's cell, and the magnetosomes were assigned according to [11] and [12] and can be observed in Figure 2 and Figure 3. All the dimensions are in nanometers and respect the realistic span of *Magnetospirillum gryphiswaldense* bacteria cell.

After the geometry was created, the next step consisted of assigning the dielectric and magnetic properties to the materials at 3 GHz, as indicated in Table 1, to each computational domain, as extracted from [13]-[14].

Table 1: Dielectric and magnetic properties of each material used in the calculations

Property	Water	Magnetite (Fe ₃ O ₄)	Cytoplasm	Membrane
Complex relative permittivity	72 – 8j	5.5 - 0.95j	67.8 – 17.6j	50.7 – 16.2j
Complex relative permeability	1	1.25 - 0.72j	1	1
Density [kg/m ³]	997	5240	1050	1200

Figure 4: Meshed geometry for each domain according to their size and the frequency

Meshing the surface represented an important issue for the precision of the results. For these simulations, we chose an extra-fine mesh automatically set according to the dimensions of the geometry and to the wavelength corresponding to 3 GHz. As it can be seen in Figure 4, the smallest elements are present over the surface of magnetite crystals and in the vicinity of the curved lines where the domain changes (from water to bacterium, from bacterium cytoplasm to magnetosome), and they grow as the size is increasing.

3. Results and Discussion

Using the AC/DC module of Comsol software, respectively Heating and losses sub-module (with frequency-domain solver), we computed the following quantities: 1) Electromagnetic power loss density; 2) Total power dissipation density; 3) Magnetic losses; 4) Specific Absorption Rate (SAR) of energy deposition. The first three are expressed in W/m³, while SAR is in W/kg. The software transposed the problem from 2D to 3D to provide these values.

Since the electromagnetic power loss density, the total power dissipation density, and SAR show remarkably similar distributions over the surface of the computational domains, in the following figures, only the significant plots are presented and shortly commented.

3.1 SAR distributions

Figure 5 shows (up to down) the change of SAR distribution when we only have water, then when the empty cell is inserted in water and then when chain of magnetosomes is present or when clustered magnetosomes are present inside the cell. The representations are given as log(SAR) values due to the huge spreading of data. The highest SAR values are shown in red and the lowest are in blue. A significant increase of SAR is observed when the cell contains the magnetosomes. Also,

differences are notable in function of the spatial distribution of magnetite nanocrystals.

Figure 5: Logarithmic SAR [W/kg] values distribution for: (a) water; (b) empty bacterium in water; (c) chained magnetosomes in bacterium+water; (d) clustered magnetosomes in bacterium+water

3.2 Magnetic losses distributions

Figure 6 presents the set of distributions for the same four situations (up to down) of the magnetic losses. It is obvious that they are significant when magnetite particles are present in the cell. Magnetic losses contribute to the total power dissipation density (Q_h) in the computation domains and will show interesting differences from SAR values, as indicated in Table 2.

Figure 6: Magnetic power loss [W/m³] distribution for: (a) water; (b) empty bacterium in water; (c) chained magnetosomes in bacterium+water; (d) clustered magnetosomes in bacterium+water

3.3 A comparison of the extreme and average values of SAR and total power dissipation density in the considered situations

This simplified approach's novelty consists of considering the contribution to the heating of both the electric and the magnetic losses that may appear in a biological sample that contains ferrimagnetic material. The magnetic losses practically sum up with classical SAR - which is calculated based solely on the internal E-field strengths. Table 2 presents pairs of values for SAR and Qh, exactly to underline the differences. Practically, maximum, minimum, and average values of these two quantities are indicated, as they were calculated over the computational domains in all four situations. We notice

that at 3 GHz, total power dissipation density highly increases when the magnetite is present in the cell. Also, both SAR and Qh become the largest when magnetosomes are positioned in the form of a chain. In this set of 2D simulations, considerable simplifications were applied, the most important being that the actual cub-octahedral form of the magnetite nanoparticles in the mentioned bacteria was not modelled and that neither the geometric nor the magnetic anisotropies were embedded in the generated model. For this reason, some differences from the 3D computations and from real situations are expected. However, present results may provide a supporting point in computational knowledge regarding microwaves magnetic hyperthermia with nanoparticles.

Table 2: Extreme and average values of specific absorption rate (SAR) and total power dissipation density (Qh) over the respective computational domains

Quantities / Situation		Case a) – water	Case b) – water + empty bacterium cell	Case c) – with chain of magnetosomes	Case d) – with cluster of magnetosomes
Min values	SAR [W/kg]	$5.79 * 10^{-7}$	$2.2762 * 10^{-5}$	$9.60 * 10^{-7}$	$1.86 * 10^{-6}$
	Qh [W/m ³]	$5.77 * 10^{-4}$	$226.93 * 10^{-4}$	1.84	2.66
Max values	SAR [W/kg]	0.017	0.042	64.12	42.63
	Qh [W/m ³]	17.76	42.86	5482.60	2476.71
Average values (over whole surface)	SAR [W/kg]	$7.57 * 10^{-4}$	$32.89 * 10^{-4}$	$681.44 * 10^{-4}$	$389.69 * 10^{-4}$
	Qh [W/m ³]	0.76	3.38	72.30	41.46

4. Conclusion and outlook

Peak SAR values are three orders of magnitude larger when the cell contains magnetite nanoparticles. When they are chained, peak SAR is about 1.5 times larger than when they are agglomerated. Average SAR values are one order of magnitude larger when the bacterium cell contains magnetosomes, and again the chained arrangement shows a higher energy absorption rate than the clustered one.

Total power dissipation density shows very similar trends.

From average SAR values, we could calculate the ratio between incident energy absorption rates of the magnetic loaded versus unloaded bacterium cell. This ratio is 20.7 times higher when the magnetosomes are chained and 11.8 times higher when the magnetosomes are clustered in the cell. Similar ratios calculated for the power dissipation density in the cell show a value of 21.9 when the magnetosomes are chained and 12.6 when the magnetosomes are clustered.

Chained - versus clustered magnetosomes

practically induced an increase in both SAR and power dissipation density of 1.7 times. At an area of 18.2 % occupied by magnetosomes from the cell area, respectively of 1.5 % occupied by magnetite particles from the cell area, a significant contribution of the magnetic loss is emphasized. Even if the presented study did not provide realistic quantitative results, it clearly

demonstrates that in the GHz region, the magnetic nanoparticles' presence triggers a different response in terms of absorbed/dissipated power in a biological compartment where they are present. A further study will translate the computations in 3D geometry, increase the number of magnetite particles, and attach other specific properties.

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