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NanoBioAI: Utilizing Python to Investigate Magnetocaloric Effects in Magnetotactic Bacteria and Optimized Conditions for Thermotherapy

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Abstract

The study presented in the research work represents a multidisciplinary approach, integrating biology, nanotechnology, and artificial intelligence. It specifically highlights the use of python computational power to investigate magnetocaloric effect (MCE) in magnetotactic bacteria (MTB), a phenomenon yet to be fully understood, characterized by reversible heating and cooling effects induced by magnetic fields. MTB are unique in that they contain embedded magnetic nanoparticles ranging from 10–100 nm in diameters. These nanoparticles provide geomagnetic responsiveness and exhibit medicinal properties such as safety, non-toxicity, superior contrasts for diagnosis, and overall biocompatibility. These characteristics make MTB a promising candidate for medical applications. The python code developed as part of this study was used to examine the heat generation by MTB under magnetic fields. The goal was to optimize the heating cycles and magnetic flux for potential effective tumor eradication. The python code was able to optimize the conditions to achieve a temperature of 40°C under two scenarios: (i) the minimum magnetic flux density would be 25 µT with 20 cycles, and (ii) the minimum number of cycles at 65 µT magnetic flux density would be 3 cycles. This computational model can be further modified considering experimental factors to optimize dosing and therapy for clinical trials and treatments. This approach enhances the safety and efficacy of MTB-based thermotherapy theoretically and has the potential to reduce the cost of animal and clinical trials. Thus, the study underscores the significant role of python in advancing the field of MTB-based thermotherapy.

Keywords: MTB-based thermotherapy, nanotechnology, python code, clinical trials, magnetotactic bacteria

INTRODUCTION

Magnetotactic bacteria (MTB) are a type of prokaryotic, Gram-negative bacteria that exhibit a behavioral response to the Earth's geomagnetic field [1]. These aquatic microorganisms contain intracellular magnetosomes, which are membrane-bound nanocrystals of magnetic iron minerals [1]. These bacteria organize their magnetosomes in linear chains, creating a magnetic dipole moment that allows them to passively orient themselves and overcome thermal forces in a water environment [2]. The primary applications of these bacteria are in the fields of environmental pollutant control, remediation and medical applications [3]. The study of MTB and their response to magnetic fields has been a topic of interest in the scientific community [4, 5]. MTB are a diverse group of bacteria with the unique ability to orient themselves

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along the Earth's magnetic field lines due to the presence of magnetosomes, which are intracellular organelles containing magnetic iron mineral nanoparticles [6].

These characteristics hold promise for diverse applications across fields such as biotechnology, environmental science, and nanotechnology [4, 5]. One area that has not been extensively explored is the effect of heating and cooling cycles induced by magnetic fields on MTB. The magnetocaloric effect, a reversible phenomenon wherein certain materials warm up under the influence of a magnetic field and cool down upon its removal, has been extensively documented [7, 8]. However, its occurrence in biological systems such as MTB is not well-understood [7, 8].

The magnetocaloric effect (MCE) is a reversible change in the entropy of a magnetic material under isothermal conditions or its temperature under adiabatic conditions due to a change of the external magnetic field [4, 5, 9]. The degree of temperature alteration is contingent upon the unique characteristics of the material and the intensity of the magnetic field applied. Additionally, these magnetosomes hold potential for a variety of applications in targeted cancer treatments, such as magnetic hyperthermia, localized drug administration, and tumor surveillance. Moreover, the entirety of MTB presents itself as a promising candidate for cancer therapy, leveraging their inherent self-propulsion via flagella and navigational guidance facilitated by their magnetosome chains. Envisaged as nanorobots, MTB can be directed and controlled by external magnetic fields, naturally gravitating toward hypoxic regions like tumor sites, while retaining both therapeutic and imaging capabilities of isolated magnetosomes. Furthermore, unlike many bacteria currently under clinical trial for cancer treatment, MTB is non-pathogenic and can be genetically modified to deliver and/or express specific cytotoxic compounds [10]. Studies in cell cultures and murine models have demonstrated that applying a rotating magnetic field to the tumor enhances the bacteria's ability to traverse the vascular barrier near the cancerous growth. In the context of MTB, one study has shown that under an alternating magnetic field, the magnetic response of the magnetic nanoparticles in MTB can produce an elevation of the temperature in the tumor, with a local increase in temperature around 4–7°C [11]. This is used for hyperthermia treatment in cancer therapy [11]. The use of MTB as a magnetocaloric material is a novel concept and, to the best of my knowledge, there are no specific studies or literature that provide data on the exact amount of temperature change that can be achieved using MTB in this way.

Artificial intelligence has been revolutionizing all value chains and every aspect of life and democratizing its used by means of prompting and tokenization [12, 13]. Python, with its extensive range of libraries like NumPy, SciPy, Matplotlib, scikit-learn, TensorFlow, PyTorch and BioPython, has been a pivotal tool in advancing medical research in medical diagnostics, hospital operations, genomic studies, drug discovery, and predictive prognosis [14, 15].

The present research work aims to study the heating cycles induced by magnetic fields on MTB using python, a powerful programming language widely used in scientific computing. The study will involve applying magnetic fluxes for various cycles to MTB, measuring the resulting increase in temperature and results will be optimized to identify optimal heating cycles and magnetic flux required to raise the temperature 20 to 40°C which is sufficient to kill the tumor cells without harming normal cells significantly. This research enhances our comprehension of the magnetocaloric effect (MCE) within biological systems through the utilization of Python programming.

STUDY DESIGN

Creating a python code that can mimic heating using magnetic field of a certain flux and create outcome in terms of heating is achieved as a function of (i) number of cycles of the magnetic field and (ii) various magnetic fluxes for single cycle. This study assumed that a fixed number of bacterial CFU are placed is a fixed dimension of container to avoid these issues in the experimental design. According to the literature, MTB react to the geomagnetic field, which typically ranges from 25 to 65 μT in magnetic flux density. Hence, any externally applied magnetic field exceeding this intensity could potentially override the geomagnetic field and efficiently guide the cells.

RESULTS AND DISCUSSION

Microstructure of MTB

MTB are diverse, motile prokaryotes found across the globe, are known for biomineralizing a unique organelle known as the magnetosome [16]. This magnetosome is characterized by a nanosized crystal composed of a magnetic iron mineral, encapsulated within a lipid bilayer membrane [16]. In the majority of MTB, these magnetosomes are arranged in well-ordered chains. This chain of magnetosomes impart a behavior to the cell akin to a motile, miniature compass needle, enabling the cell to align and swim in parallel to magnetic field lines [16]. MTB are usually mineralized by either iron oxide magnetosomes containing crystals of magnetite (Fe_3O_4), or iron sulfide magnetosomes containing crystals of greigite (Fe_3S_4). Figure 1 provides transmission electron microscopy (TEM) images of MTB (containing magnetite nanoparticles particles) studied by Lohße *et al.* [17]. The scale bar in Figure 1A is 400 nm, and in Figure 1(B and C) is 50 nm.

Figure 1A depicts the TEM micrograph of MTB with embedded magnetic nanoparticles aligned in a certain direction. Figure 1B depicts the enlarged view of the aligned magnetic nanoparticles and Figure 1C shows the enlarged view of a few nanoparticles form the same chain giving an idea about their nanosized diameters.

The magnetically guided locomotion of these aquatic bacteria does not entail pulling the bacteria along geomagnetic field lines in a manner akin to how a magnet attracts metal; rather, it merely aligns their single-celled bodies with these lines. The bacteria must still wiggle their flagella to move forward or backward [18] and exhibit the unique ability to orient along the magnetic field lines which is known as “magnetotaxis” [19]. MTB can survive in natural extreme environments with a wide temperature range from 0 to 70°C [20, 21, 22]. Some of the MTB strains have exhibited maximum survival and growth at temperature about 63°C [23]. The precise temperature range can fluctuate based on the particular strain of bacteria [23].

Thermotherapy or photothermal therapy, a treatment modality (using 10–100 nm magnetic particles) that raises the temperature at the tumor site to 41–43°C, can damage and kill cancer cells while sparing benign cells [24–26]. It enhances cancer cell sensitivity to chemotherapy or radiation, promotes cyclic suicide of residual cancer cells post-treatment, and boosts immune system efficiency by activating immune cells and making tumor cells more susceptible to destruction [24–26].

MTB and their magnetosomes have multiple advantages over nano functionalized magnetic particles used in thermotherapy or photothermal therapy, as follows:

Non-Pathogenic [27]

In contrast to the majority of bacteria currently undergoing investigation in clinical trials for cancer therapy, MTB are non-pathogenic, yet they could potentially undergo modifications to facilitate the delivery and expression of specific cytotoxic agents.

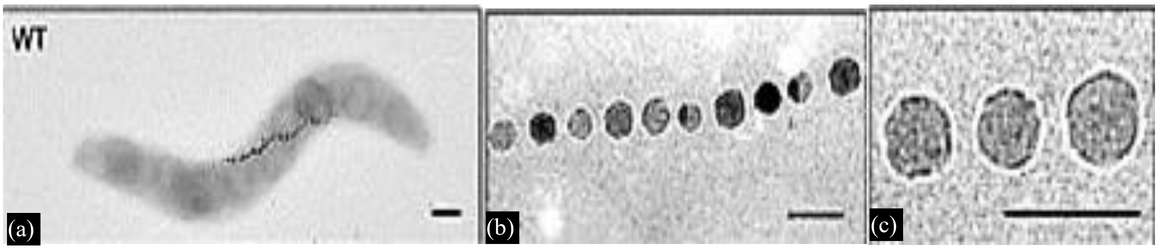


Figure 1. TEM micrograph of MTB: Figure A is magnetosome with embedded particles (scale bar 400 nm), and Figure 1B are nanoparticles and 1C are enlarged view of some nanoparticles (scale of 50 nm) [17].

Higher Heating Efficiency [27, 20]

Magnetosomes from MTB have been found to have high heating efficiency, making them an effective alternative for the development of magnetic hyperthermia therapy.

Heat Reversibility [28]

Magnetotactic bacteria warm up when an alternating magnetic field is applied due to changes in their internal state, which releases heat. When the magnetic field is removed, the bacteria can return to their original state, reabsorbing the heat or dissipated to surrounding environment, and returning to their original temperature. This property is crucial for their potential use in targeted hyperthermia treatments for diseases like cancer.

High Purity Levels [20, 29]

The biologically controlled mineralization of magnetosomes ensures high purity and perfect magnetosome crystal lattice, whereas synthetic nanoparticles synthesized by the method of coprecipitation are often impure and have structural defects. In addition to being of high purity, magnetosomes are non-pyrogenic and devoid of bacterial endotoxins and used in prostate cancer therapy.

Narrow Size Distribution [17]

Magnetosomes have a narrow size distribution when they are grown under optimal conditions. This is beneficial for magnetic hyperthermia as the size of the particles is one of the relevant properties.

Self-Propulsion and Guidance [30, 31]

The entirety of MTB holds promise as potential candidates for cancer treatment, leveraging the self-propulsion capability of their flagella and the guiding function of their magnetosome chain. Conceptualized as nanobots, MTBs can be directed and controlled by external magnetic fields, naturally navigating towards hypoxic regions like tumor sites, all while maintaining the therapeutic and imaging properties of isolated magnetosomes.

Thermally Stable Magnetic Moment [20]

Magnetosomes consist of sizable single-domain nanoparticles, resulting in a magnetic moment that remains thermally stable even at physiological temperatures.

Better MRI Contrast Agents [20]

The utilization of magnetosomes as contrast agents in magnetic resonance imaging (MRI) surpasses that of chemically synthesized nanoparticles. These benefits render MTB and their magnetosomes a highly promising avenue of exploration for cancer treatment. Nonetheless, further investigation is imperative to comprehensively grasp and capitalize on these advantages for clinical utilization.

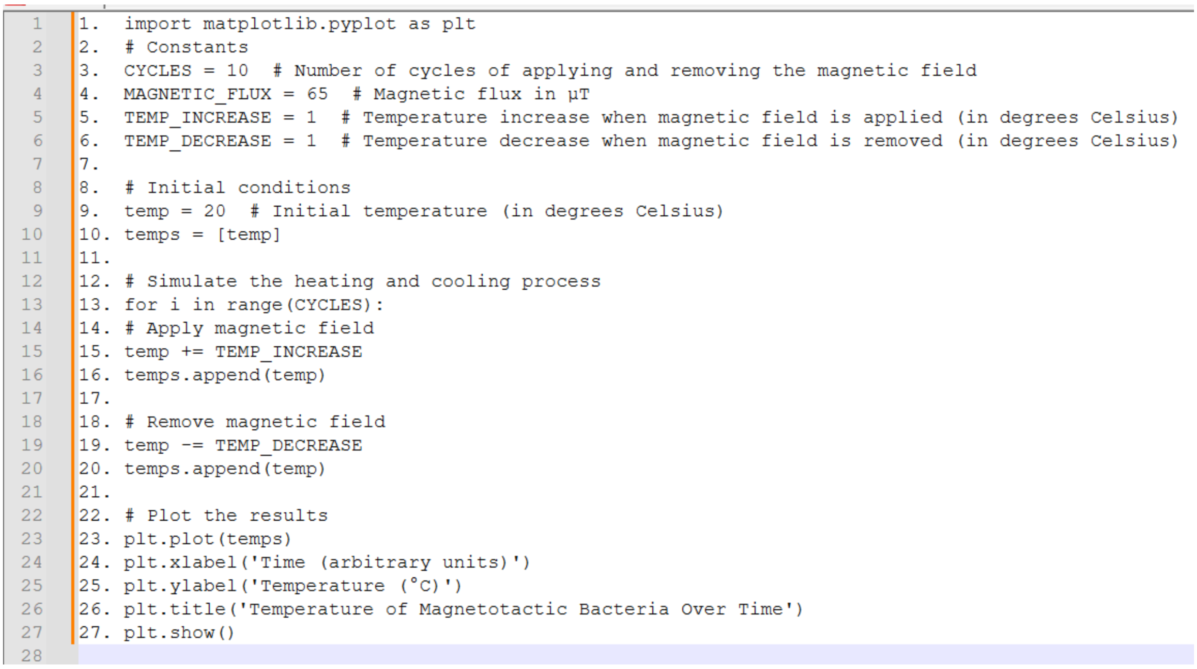
Python Code for Repeating Magnetic Heating Cycles to Increase Temperature

Python code that simulates the heating process due to different cycles is as shown in Figure 2. This code assumes that the temperature increase is linearly proportional to the cycles, with a magnetic flux density of 65 μT causing a temperature increase of 4–7°C [11].

Python code for repeating magnetic heating cycles to increase temperature is given in Figure 2.

Results from the python for repeating magnetic heating cycles to increase temperature is provided in Table 1.

Table 1 shows that the temperature increases linearly with number of cycles and around 13 cycles are required to reach 40°C which may potentially help irradicate tumor.



```
import matplotlib.pyplot as plt
# Constants
CYCLES = 10  # Number of cycles of applying and removing the magnetic field
MAGNETIC_FLUX = 65  # Magnetic flux in µT
TEMP_INCREASE = 1  # Temperature increase when magnetic field is applied (in degrees Celsius)
TEMP_DECREASE = 1  # Temperature decrease when magnetic field is removed (in degrees Celsius)

# Initial conditions
temp = 20  # Initial temperature (in degrees Celsius)
temps = [temp]

# Simulate the heating and cooling process
for i in range(CYCLES):
# Apply magnetic field
temp += TEMP_INCREASE
temps.append(temp)

# Remove magnetic field
temp -= TEMP_DECREASE
temps.append(temp)

# Plot the results
plt.plot(temps)
plt.xlabel('Time (arbitrary units)')
plt.ylabel('Temperature (°C)')
plt.title('Temperature of Magnetotactic Bacteria Over Time')
plt.show()
```

Figure 2. Python code for repeating magnetic heating cycles to increase temperature.

Table 1. Magnetic heating cycles.

Cycle Number	Temperature Before Heating (°C)	Magnetic Field Applied: 65 µT	Temperature Range After Heating (°C)
1	20	21	28
2	21	22	29
3	22	23	30
4	23	24	31
5	24	25	32
6	25	26	33
7	26	27	34
8	27	28	35
9	28	29	36
10	29	30	37
11	30	31	38
12	31	32	39
13	32	33	40

Python Code for Various Fluxes to Increase Temperature

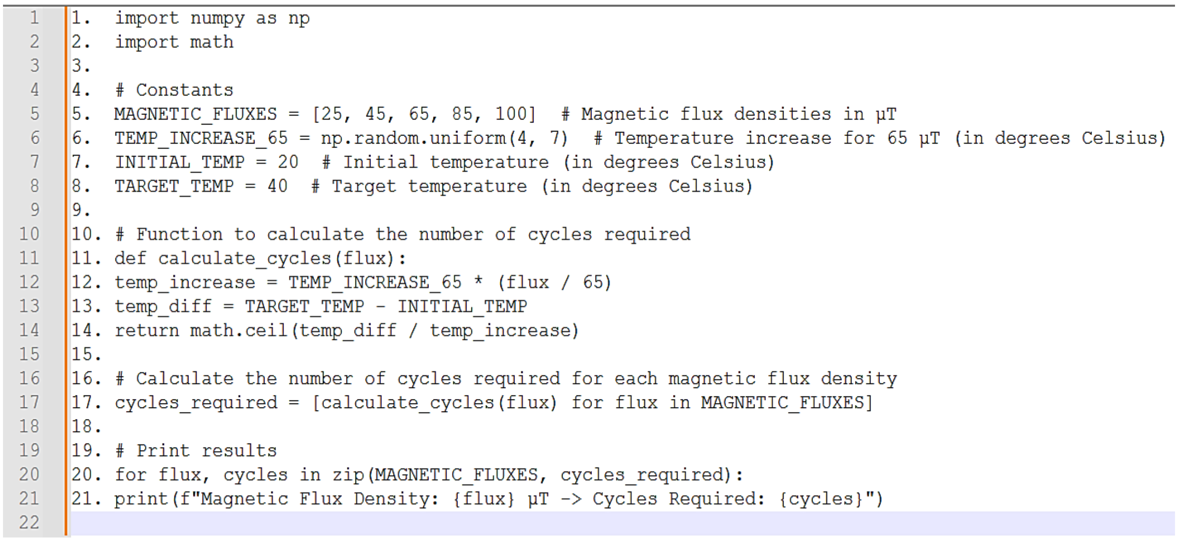
Python code that simulates the heating process due to different magnetic flux densities is as follows:

This code assumes that the temperature increase is linearly proportional to the magnetic flux density, with a magnetic flux density of 65 µT causing a temperature increase of 4–7°C. Python code for various fluxes to increase temperature is given in Figure 3.

This code calculates the temperature increase for each magnetic flux density and provides the results as shown in Table 2. Table 2 shows that for a one cycle, magnetic flux of 545.5 µT is required to reach 40°C that may potentially eradicate tumors.

Table 2. Magnetic flux density.

Magnetic Flux Density (µT)	One Cycle	Temperature Range After (°C)
25	1.54	8.54
45	2.77	9.77
65	4	11
85	5.23	12.23
100	6.15	13.15
120	7.38	14.38
138.5	8.517	15.517
157	9.654	16.654
175.5	10.791	17.791
194	11.928	18.928
212.5	13.065	20.065
231	14.202	21.202
249.5	15.339	22.339
268	16.476	23.476
286.5	17.613	24.613
305	18.75	25.75
323.5	19.887	26.887
342	21.024	28.024
360.5	22.161	29.161
379	23.298	30.298
397.5	24.435	31.435
416	25.572	32.572
434.5	26.709	33.709
453	27.846	34.846
471.5	28.983	35.983
490	30.12	37.12
508.5	31.257	38.257
527	32.394	39.394
545.5	33.531	40.531



```
1.  import numpy as np
2.  import math
3.
4.  # Constants
5.  MAGNETIC_FLUXES = [25, 45, 65, 85, 100]  # Magnetic flux densities in µT
6.  TEMP_INCREASE_65 = np.random.uniform(4, 7)  # Temperature increase for 65 µT (in degrees Celsius)
7.  INITIAL_TEMP = 20  # Initial temperature (in degrees Celsius)
8.  TARGET_TEMP = 40  # Target temperature (in degrees Celsius)
9.
10. # Function to calculate the number of cycles required
11. def calculate_cycles(flux):
12. temp_increase = TEMP_INCREASE_65 * (flux / 65)
13. temp_diff = TARGET_TEMP - INITIAL_TEMP
14. return math.ceil(temp_diff / temp_increase)
15.
16. # Calculate the number of cycles required for each magnetic flux density
17. cycles_required = [calculate_cycles(flux) for flux in MAGNETIC_FLUXES]
18.
19. # Print results
20. for flux, cycles in zip(MAGNETIC_FLUXES, cycles_required):
21. print(f"Magnetic Flux Density: {flux} µT -> Cycles Required: {cycles}")
```

Figure 3. Python code for various fluxes to increase temperature.

Optimization of Magnetic Flux and Magnetic Cycles to Achieve 40°C

Python code for optimization of magnetic flux and magnetic cycles to achieve 40°C is given in Figure 4. The code provides the conditions to achieve 40°C to potentially eradicate tumors as (i) the minimum magnetic flux density would be 25 µT with 20 cycles, and (ii) the minimum number of cycles at 65 µT magnetic flux density would be 3 cycles.

The above results can be explained as follows.

- The initial temperature is 20°C.
- The increase in temperature per cycle for a magnetic flux density of 65 µT is between 4 and 7°C.
- For magnetic flux densities less than 65 µT, the temperature rise will be statistically less, and for higher flux densities, the temperature rise will be higher.

Given these conditions, to achieve a temperature of 40°C from an initial temperature of 20°C, we need an increase of 20°C.

Number of cycles required

If we consider the maximum temperature increase per cycle (7°C at 65 µT), we will need at least 3 cycles (as 7°C×3 cycles=21°C, which is just over the required 20°C increase).

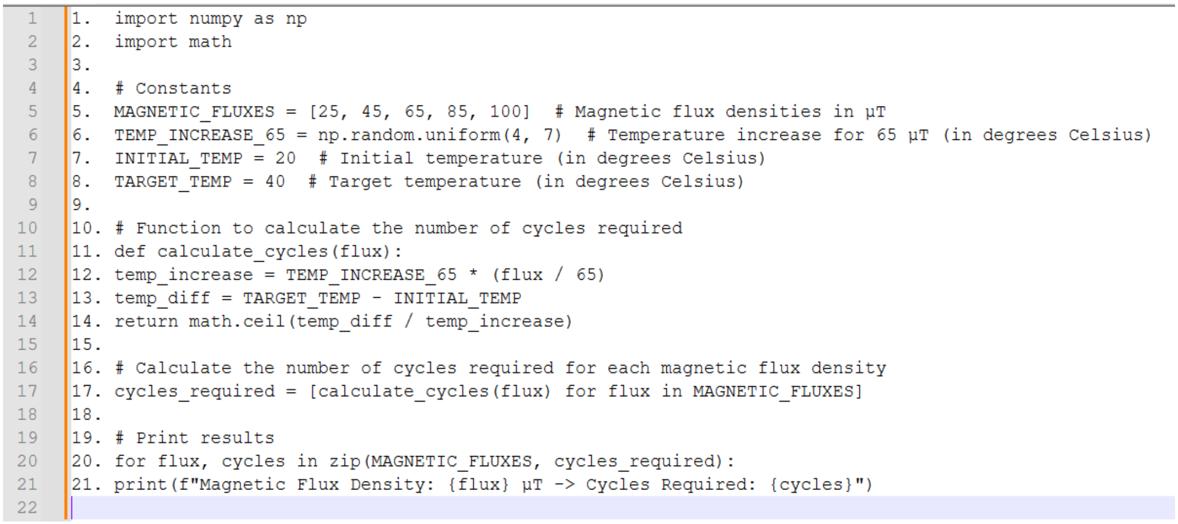
If we consider the minimum temperature increase per cycle (assuming 1°C increase at 25 µT), we will need 20 cycles (as 1°C×20 cycles=20°C).

Therefore, the minimum magnetic flux density that could achieve a 40°C temperature would be 25 µT with 20 cycles, and the minimum number of cycles at 65 µT magnetic flux density would be 3 cycles.

Study Constraint

Please note that this is a simplified model and does not consider additional factors that would be important in a real-world scenario, such as the specific properties of the bacteria and the magnetic field, heat transfer to the surrounding environment, and the effects of repeated heating and cooling on the bacteria. For a more accurate model, we need to incorporate these factors and potentially use more sophisticated modelling techniques.

It is crucial to highlight that although these discoveries show promise, additional research is required to thoroughly grasp the potential advantages and drawbacks of employing MTB in cancer therapy.



```
import numpy as np
import math

# Constants
MAGNETIC_FLUXES = [25, 45, 65, 85, 100]  # Magnetic flux densities in µT
TEMP_INCREASE_65 = np.random.uniform(4, 7)  # Temperature increase for 65 µT (in degrees Celsius)
INITIAL_TEMP = 20  # Initial temperature (in degrees Celsius)
TARGET_TEMP = 40  # Target temperature (in degrees Celsius)

# Function to calculate the number of cycles required
def calculate_cycles(flux):
temp_increase = TEMP_INCREASE_65 * (flux / 65)
temp_diff = TARGET_TEMP - INITIAL_TEMP
return math.ceil(temp_diff / temp_increase)

# Calculate the number of cycles required for each magnetic flux density
cycles_required = [calculate_cycles(flux) for flux in MAGNETIC_FLUXES]

# Print results
for flux, cycles in zip(MAGNETIC_FLUXES, cycles_required):
print(f"Magnetic Flux Density: {flux} µT -> Cycles Required: {cycles}")
```

Figure 4. Python code for optimization of magnetic flux and magnetic cycles to achieve 40°C.

Future Research

MTB has great efficiency in heating for tumor cell inhibition and their heat efficiency in alternating magnetic fields is affected by the hysteresis loop [28]. Also, ongoing research is being conducted on the MCE of MTB, with the aim of enhancing their magnetocaloric safety and efficacies that is essential for clinical trials and cancer treatments. However, a few challenges that need to be addressed are such as reducing the heat exchange time between the bacteria and their surrounding environment, implementing smart thermal control through integrated thermal switches, and minimizing the undesirable magnetic hysteresis loss. When MTB is cultured in a specific medium, the specific absorption rate of MTB cells can be significantly higher than that of current commercial magnetic particles [28]. Additional research is required to increase the mechanical stability of the bacteria, enhance the MCE for low-applied field values, and broaden the operational temperature range.

Addressing these challenges, further studies are exploring the use of cascade systems composed of MTB [28]. After studying all the parameters mentioned above experimentally, the python codes can be modified to optimize the dosing (the amount of MTB required per the weight of the patient), and therapy parameters (magnetic flux and cycles) to maximize the safety and efficacy of thermotherapy [32]. Such a python based theoretical analysis may help to optimize and speed up the animal model and clinical trial experiments and reduce cost of clinical trials and the MTB thermotherapy in future.

CONCLUSION

The study successfully demonstrates the potential of a multidisciplinary approach combining biology, nanotechnology, and artificial intelligence to advance medical applications. By utilizing Python to investigate the magnetocaloric effects in magnetotactic bacteria (MTB), the research provides new insights into the optimization of MTB-based thermotherapy. The computational model developed in Python effectively optimized heating cycles and magnetic flux density to achieve a therapeutic temperature of 40°C, identifying two key scenarios for minimal magnetic flux and cycle count. This model not only enhances the theoretical understanding of MTB's medicinal properties but also has practical implications for improving the safety, efficacy, and cost-effectiveness of MTB-based treatments. The results pave the way for future modifications of the model to incorporate experimental factors, ultimately aiding in the optimization of dosing and therapy for clinical trials. Thus, the study highlights the crucial role of Python in innovating and refining MTB-based thermotherapy, promising a significant impact on the field of medical nanotechnology.

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