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RESEARCH PAPER

Evaluation of the effect of gold and iron oxide nanoparticles dispersed on the bolus in radiation therapy by using Monte Carlo simulation

MaryamYaftian [1], Elham Saeedzadeh [1], Hossein Khosravi [2]*, EhsanMohammadi [3]

[1]Department of Radiation Medical Engineering , Science and Research branch, Islamic Azad University, Tehran, Iran
[2]Department of Radiology, School of Allied Medical Sciences, Hamadan University of Medical Sciences, Hamadan, Iran
[3]Cancer Institute, Imam Khomeini Hospital, Tehran University of Medical Sciences, Tehran, Iran

ABSTRACT

Objective(s): The aim of this study was to determine the entrance skin dose distribution for breast cancer patients who undergo radiotherapy in the presence of bolus containing gold and Fe_3O_4 nanoparticles to evaluate and compare the changes in dose distribution.

Materials and Methods: Gold and Fe_3O_4 nanoparticles can increase the rate of photoelectric, Compton, and pair production absorption of x-ray photons. Nanoparticles were simulated in the bolus, over the skin of a breast phantom, by the exertion of MCNPX Monte Carlo code. The skin dose was also experimentally measured by using a bolus that contained homogeneously distributed Fe_3O_4 nanoparticles on the surface of a slab phantom and an advanced Markus chamber.

Results: A significant skin dose enhancement was obtained for the case that 25 nm gold and Fe_3O_4 nanoparticles with 3% concentration were uniformly distributed in the bolus. However, increased concentration of nanoparticles in the bolus will increase the skin dose.

Conclusion: It is concluded that using nanoparticles in the bolus leads to a significant skin dose enhancement for 6 MV x-ray photons. Furthermore, this study suggested that, less thick blouses may provide the same dose distribution.

Keywords: *Bolus, Breast cancer, MCNPX Monte carlo code, Nanoparticles, Skin dose*

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INTRODUCTION

Undoubtedly, increasing the received dosage of drug by cancer cells can significantly improve the results of a cancer treatment, which can be accomplished by the exertion of nanoparticles as a radiation sensitizing agent in cancer cells. Along with the enhancing impact of their introduction to medical fields on treatment methods, the wide applications, small size, and large surface-to-volume ratio of nanoparticles can provide more radiation in the area of tumors and to some extent reduce their effects on the surrounding healthy tissues by protecting them from radiation damage [1- 3].

Gold nanoparticles (GNPs) are the best choice for these processes due to their compatibility with biological environments and low toxicity.

The collision of a photon with a gold atom, due to its high atomic number (high Z), produces a large number of X-ray electrons, which can also generate a high dose by its short-range [4].

Bolus is a naturally or synthetically developed material that acts as a layer of tissue to provide more effective treatment for superficial lesions. The very first report on the application of bolus was made by Jungling in early 1920s and is still used in radiation therapy. This type of therapy is often performed to treat superficial lesions in cancer patients, which are located on or near the surface or cracks of the patient's skin. Meanwhile, a bolus can deliver the dose to near the surface of

* *Corresponding author: Email: h.khosravi@umsha.ac.ir*
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patient's skin before the megavolt photon beams reach electron equilibrium [5].

In recent years, numerous studies were conducted on the application of nanoparticles in radiotherapy by experimental trials and Monte Carlo simulations. Despite the ongoing debate over the idea of increasing the applied dosage by elements with high atomic numbers for decades, scientists were prompted to further assess the various applications of nanoparticles in radiation therapy due to their compatibility with biological systems. The results of all studies in this field confirmed the impact of increasing the applied dosage on reaching the tumor in radiation therapy by nanoparticles. However, there are controversial results from the interaction of radiant energy with the size of gold nanoparticles as well. The most effective parameters in Monte Carlo simulation in regards to facilitating a further extension in the dosage implicate large nanoparticles, high molar concentration, and low energy X-ray or gamma photons [5-8].

In radiotherapy, ionizing radiation such as X-rays, gamma rays, and high-energy particles are widely used to treat cancerous tumors in solid form. Unfortunately, ionizing radiation is not able to distinguish cancer cells from healthy cells. Therefore, healthy tissue is damaged by radiation therapy to eradicate cancer cells. The main purpose of using nanoparticles in specific tumors in radiation therapy is to improve the outcome of radiation therapy by increasing the toxicity of tumors and decreasing it for healthy cells [9-12]. Among different nanoparticles, preclinical studies have been performed on gold nanoparticles and their sensitivity to different photon beams.

One of the studies of Cho et al. was conducted on the feasibility of using gold nanoparticles as an aid in low-energy radiation therapy by Monte Carlo calculations, which implicated the application of X-ray with 50 KVp energy and 125I- and 169-Yb brachytherapy glasses. They also performed macroscopical calculations related to dose-increasing factors with and without the presence of gold nanoparticles in the tumor. They reported an increase of more than 40% in the dosage for their exerted radiation sources in the presence of gold nanoparticles that contained the dimensions of 1.9 nm [13].

Moreover, Choi et al. attempted to study the feasibility of using iron oxide nanoparticles as an adjunct to PAT radiation therapy in superficial tumors of mice. Accordingly, next to the application of PAT for the treatment of CT26 tumor cells, tumor mice CT26 was also used through the application of a 13-nm FeO NP diameter to be exposed to 7.1 kV near the Fe K-edge by synchrotron X-ray irradiation. Cell survival was determined by MTT assay and tumor regression was performed to test the in vivo model. Finally, the results of PAT-treated groups were compared with X-ray control groups. According to the results of this study, an iron oxide nanoparticle with a relative concentration of iron and 10 g of monochromatic X-ray can increase the therapeutic effects. Considering the severe attenuation of 7.1 Kev X-rays in tissues, the promising potential of FeO NP-PAT can be suggested as a strong treatment option for superficial skin malignancies such as the recurrence of breast cancer chest wall [9].

In this study, we exploited the effect of gold nanoparticles (GNPs) and iron oxide to provide a sufficient amount of gold and iron oxide through a uniformed distribution in the bolus adjacent to superficial lesions and breast tumor, while lacking any evident toxicity for increasing the dosage and eradicating the tumor. We also evaluated the increasing rate of dosage in breast therapeutic volume. The applied energy in this research was 6 MV. Several softwares such as GEANT4, MCNP, BEAMnrc, and EGSnrc , which are designed to perform calculations based on the Monte Carlo method, were used for the simulation. MCNP was considered as a suitable software for our investigation due to its ability to simulate the transfer of photons and electrons over a wide range of energies [14].

MATERIALS AND METHODS

The objective of this study was to investigate the energy optimization of photons colliding with gold and iron oxide nanoparticles in different dimensions , as well as to calculate the increasing rate of dosage through the usage of Monte Carlo method. Furthermore, we exploited the supremely accurate and extensive library of cross-sections of MCNPX simulation software to calculate the probabilities of nuclear interactions occurrence. For different materials used in the program, the mcplib22 and el032 cross-sectional libraries were exerted for photons and electrons, respectively. Lastly, certain softwares such as MATLAB or EXCELL were used to analyze the data of Monte Carlo simulation and draw the same dose curves and related tables.

MCNPX code

This code was first introduced in 1977 under the label of MCNP and in 2000, the 4C version entered the market, which was followed by the designs of X, 2.6X, and 5 versions. The energy range of electron and photon transport in Monte Carlo MCNP code extends from 1 kV to 100 MeV, which at low energies can facilitate the accurate design of photoelectric characteristics and Auger electrons and X-rays. Also, the prominent feature of MCNPX code is the construction of voxels, which spatially distributes large volumes into smaller voxels in three dimensions, while the tally calculates the energies of these small voxels [15]. This study was done by the usage of MCNPX version, while the code preparation required the definition of its parameters in an organized order, each of which is often referred to as a "card".

Next to the application of lattice command to draw our iterative structures, the exerted cards for the cell included the body card, breast card, bottom card, top card, middle card (for skin), bolus cube card (test volume), environment card, and Outside environment card. Additionally, the existing nanoparticles inside the bolus, which were observed in the form of spherical volumes, were calculated at the tested concentrations and radii, which was Coded through the nanoparticle meshing technique. In regards to the surface cards, we exerted cylindrical, spherical cards, and surfaces for the six-dimensional cube volume of the bolus along with spherical cards for nanoparticles. This research exploited two categories of iron oxide and gold nanoparticles for its simulations,which were performed in p and e modes of f8 and f*8 tally card in the number of 1,000,000 particles.

Simulation of cell geometry and breast phantom

Subsequent to simulating a simple phantom, the breast geometry was embedded with a radius of 2.5 cm, the skin with a thickness of 2 mm, and the bolus with a thickness of 1 cm. Then, the bolus at irradiation site was set out as a cube to facilitate the assessment of model and proceed by performing the simulation. This cube with the dimensions of 1 cm 1 cm× 1 cm was located in the center distance of tangent bolus with a radiating angle in the breast phantom (Fig. 1).

The bolus cube was made of soft tissues with an equivalent density. The composition of soft tissue was consisted of 1.10% hydrogen, 1.11% carbon, 6.2% nitrogen, and 2.76% oxygen.

To simulate the bolus, it was first segmented to the dimensions of 1 cm × 1 cm × 1 cm, which can be observed in Fig. 2.

Succeeding to the step of bolus segmentation, which is calculated based on the concentration and dimensions of gold nanoparticles, spherical gold nanoparticles were placed inside these segments. Fig. 3 exhibits the general geometry with the ideal distribution of gold nanoparticles.

Uniform distribution models of gold and iron oxide nanoparticles

In this section, gold nanoparticles in a concentration of 1% and 3% by weight with the dimensions of 25, 40, and 50 nm were used next to the application of iron oxide nanoparticles (Fe_3o_4) with a radius of 25, 40, and 50 nm and a concentration of 3%. The most ideal situation occurs when it is assumed that the nanoparticles are distributed evenly throughout the tumor, in which every part of the bolus faces the same distribution in terms of different distribution of nanoparticles

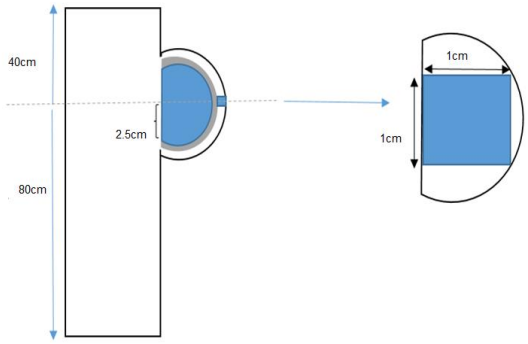


Fig. 1. the position of cube at the bolus in phantom geometry

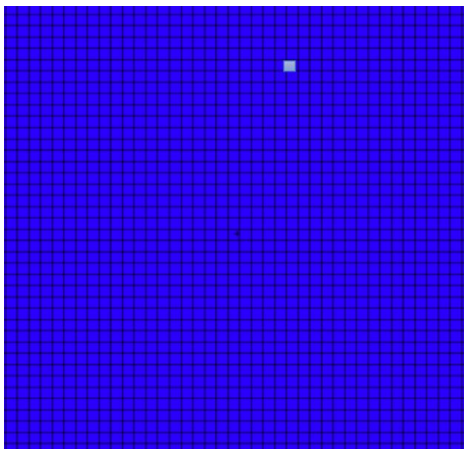


Fig. 2. of the bolus with dimensions of 1 cm × 1 cm × 1 cm that was segmented into cubes

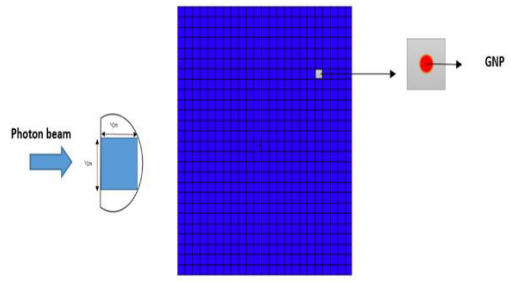


Fig. 3. Overview of geometry with ideal distribution of gold nanoparticles in bolus

and the concentration difference in the center and surface, which may be absent between the center and its surface as well. Therefore, the following equation can configure the rate of this distribution by distributing it on the surface of bolus, since this factor is the same everywhere with the number 1, while being number zero outside the bolus.
According to the equation (2-1);

$$D_{uni\ formy\ GNP}(r) = \begin{cases} D=1 \quad if \quad 0 \leq r \leq A \\ D=0 \quad if \quad r > A \end{cases} \qquad (2\text{-}1)$$

(2-1) - A refers to the dimensions of bolus, r represents the distance from the center to the surface of bolus, and D stands for the amount of gold nanoparticles distribution.

Estimation of dose increase

To estimate the dose increase in accordance to the Source Surface Distance (DEF) definition (Equation 2-2), the amount of breast dose within the phantom geometry was initially calculated in the absence of gold and iron oxide nanoparticles. Then, the gold and iron oxide nanoparticles in concentrations of 1 and 3% and with different dimensions of 25 and 40 and 50 nm were applied to calculate the dose on bolus and also measure the DEF value of whole tumor through Equation (2-2).

DEF= Dose with presence of nanoparticle/Dose without presence of nanoparticle (2-2)

This research implicated the energy value of 6 MV, while the calculation error in the simulation was considered up to 0.0001.

Estimation of dose increase (DEF) in the case of uniform distribution of nanoparticles in the bolus volume

In order to simulate the uniform distribution of gold nanoparticles throughout the bolus, a lattice card and a grid property was initially used to divide a cubic bolus with the dimensions of 1 cm × 1 cm × 1 cm into smaller cubes and place spherical gold nanoparticles inside them. The exerted method for calculating the number of gold nanoparticles in the bolus lattice geometry is presented below.

Assuming that the gold nanoparticles are spherical, the number of nanoparticles can be determined through the following equations.

$$V_{cluster} = NV_{atom} \qquad (2\text{-}3)$$

$$\frac{4}{3}\pi(R_{cluster})^3 = N\frac{4}{3}\pi(R_{atom})^3 \qquad (2\text{-}4)$$

Where V is the volume of cluster or atom, R stands for the radius of cluster or atom, and N refers to the total number of atoms inside the cluster. The following equations are the rewritten states of the mentioned relationships:

$$R_{Cluster} = N^{1/3} R_{atom}$$

$$R_{gold\ atom} \sim 0.137\ nm$$

Every nanoparticle of this research contained specific dimensions and the concentrations of 1% and 3%. As it is presented in Tables 1, 2), the size of grades varies in accordance to the dimensions of nanoparticles.

The program was run separately for the transport of 10^6 × 2 particle to perform the calculations and simulate the program for each of the nanoparticles with different dimensions and the assigned concentrations. The calculation of the DEF of skin surface was conducted by determining the amount of breast absorption dose of the two cases in the presence and absence of gold nanoparticles and proceeding by configuring the amount of DEF through Equation (2-2).

RESULTS

In this study, the rate of dose increase in the chest and bolus, involved in the form of a cube with a volume of 1 cm^3, was designed in the central distance of bolus tangent to the radiant beam of the phantom of the chest and a photon pencil beam

Table 1. Different dimensions of grids (Location of nanoparticles) at a concentration of 3% by weight

Dimensions of grides (cm)	Dimensions of nanoparticles (nm)
5.835E-5	25
9.338E-5	40
1.16E-4	50

Table 2. Different dimensions of grids (Location of nanoparticles) at a concentration of 1% by weight

Dimensions of grides (cm)	Dimensions of nanoparticles (nm)
4.049E-5	25
6.47E-5	40
8.09E-5	50

spring located at a distance of 101.25 cm from the center. The doses of distributed Gold nanoparticles at concentrations of 1% and 3% in the bolus were calculated as well, which was followed by a dose increase factor in accordance to Equation (2-2).

Estimation of dose increase in uniform distribution model of gold nanoparticles

We carried out the process of dose increase calculations (DEF) in breast skin volume and cubic geometry volume in a bolus at the presence of nanoparticles with the dimensions of 25, 40, and 50 nm and the concentration of 1% and 3% with the energy value of 6 MV, while assuming the implication of a uniform distribution of nanoparticles, The obtained results are provided in the diagrams below (Figs. 4-9).

In conformity to these diagrams, the maximum increase in skin dose of nanoparticles in a concentration of 1% and the dimensions of 25 nm was equaled to 1.150 and for nanoparticles in a concentration of 3% with the dimensions of 25 nm was equaled to 1.165, while an increase was observed in the absorption dose as the nanoparticles concentration was enlarged.

Estimation of dose increase in bolus cube in the uniform distribution model of gold nanoparticles

The dose increase was calculated for a bolus cube with a volume of 1 cm^3 that consisted grid and gold nanoparticles with a concentration of 1 and 3% by weight and the dimensions of 25, 40 and 50 nm. An examination on the induced changes are

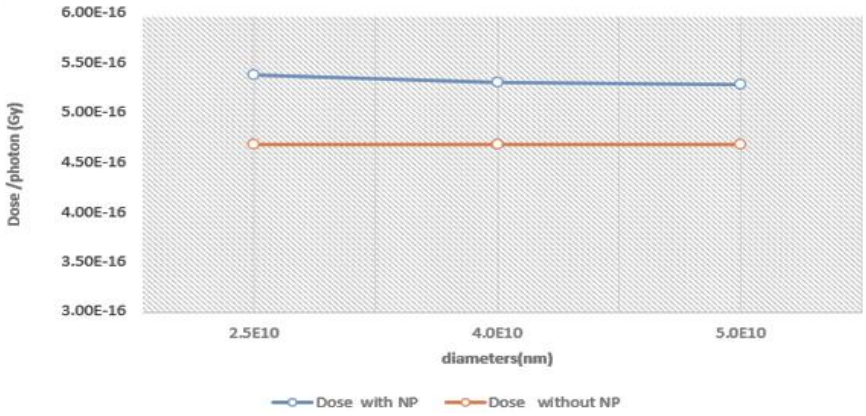


Fig. 4. The absorbed dose of skin surface in the presence and absence of nanoparticles in a concentration of 1% and 6 MV energy

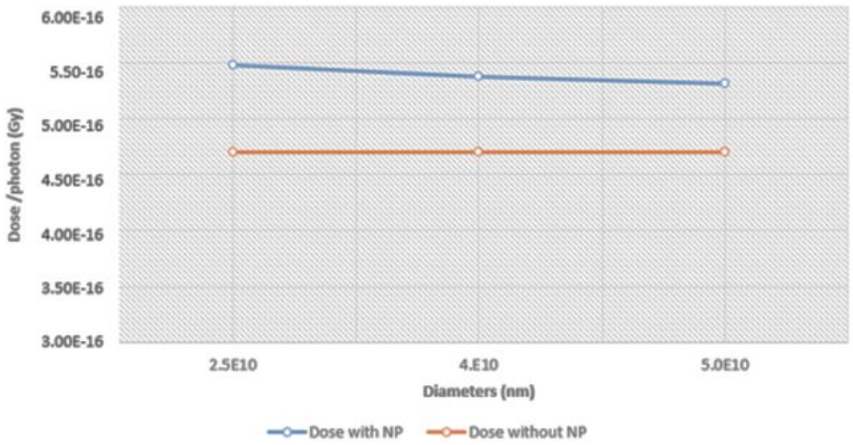


Fig. 5. The absorbed dose of skin surface in the presence and absence of nanoparticles with a concentration of 3% in 6 MV energy

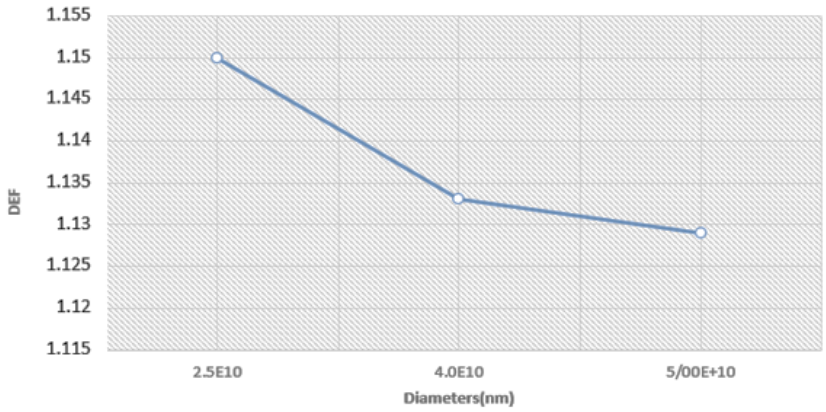


Fig. 6. Comparison of the absorbed dose of skin surface in the presence and absence of nanoparticles with concentrations of 1% and 3% in 6 MV energy

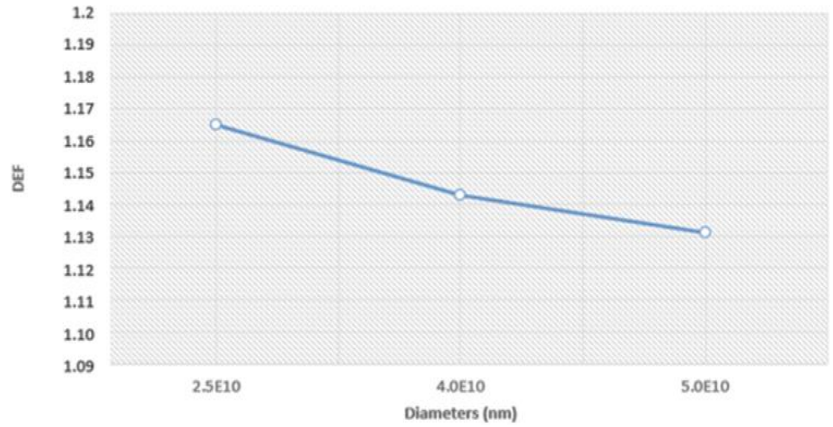


Fig. 7. Dose increase coefficient of skin surface area (DEF) in the presence of nanoparticles with a concentration of 1% in 6 MV energy

presented in the diagram below (Fig. 10-12).

According to the diagrams, the maximum value of bolus dose increase coefficient was 0.954 for nanoparticles in a concentration of 1% with the dimensions of 50 nm, and 0.970 for the nanoparticles with a concentration of 3% and the dimensions of 50 nm. Moreover, an evident extension was observed in the coefficient of dose increase as a result of enlarging

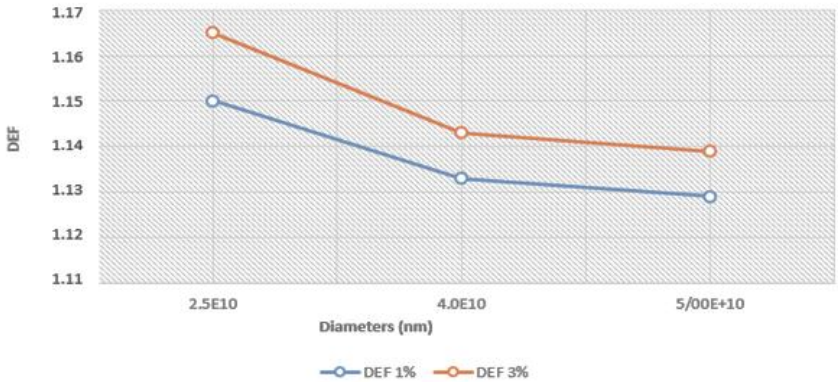


Fig.8. Increase of the skin surface absorption dose (DEF) in the presence of nanoparticles with a concentration of 3% in 6 MV energy

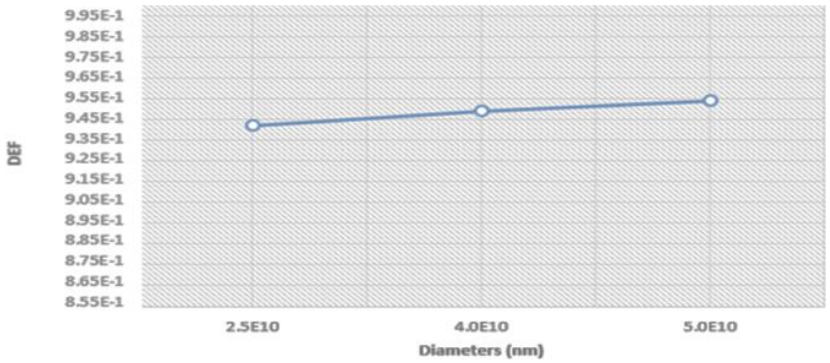


Fig. 9. Increased absorption dose (DEF) coefficient of skin surface in the presence of nanoparticles with concentrations of 1 and 3% in 6 MV energy

the applied concentration.

Estimation of dose increase in uniform distribution model of iron oxide nanoparticles (Fe_3o_4)

The results of gold nanoparticles distribution indicated the highest dose increase from nanoparticles with a radius of 25 nm at a weight concentration of 3%. In addition to calculating the dose distribution in breast skin volume by using the uniform distribution of gold nanoparticles for evaluating the effectiveness and performing a comparison with the experimental results, which will be addressed in the following, we also calculated the increasing rate of absorbed dose level of skin surface (DEF) in the presence of iron oxide nanoparticles at a concentration of 3% and presented the outcomes in below (Fig. 13 and Fig. 14).

In conformity to the diagrams, the maximum

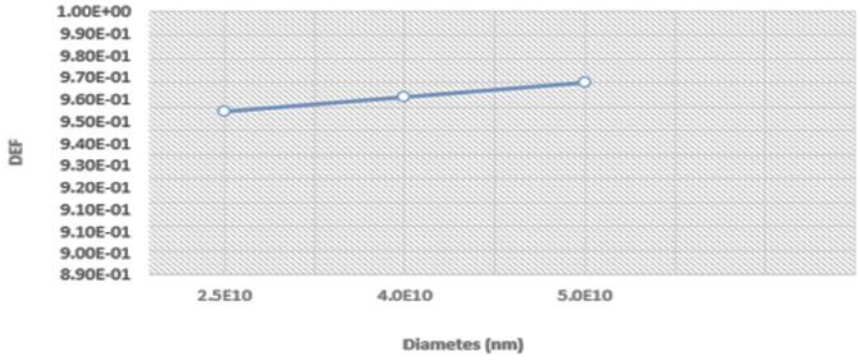


Fig. 10. Bolus absorption dose increase coefficient (DEF) in the presence of nanoparticles with a concentration of 1% with energy of 6 MV

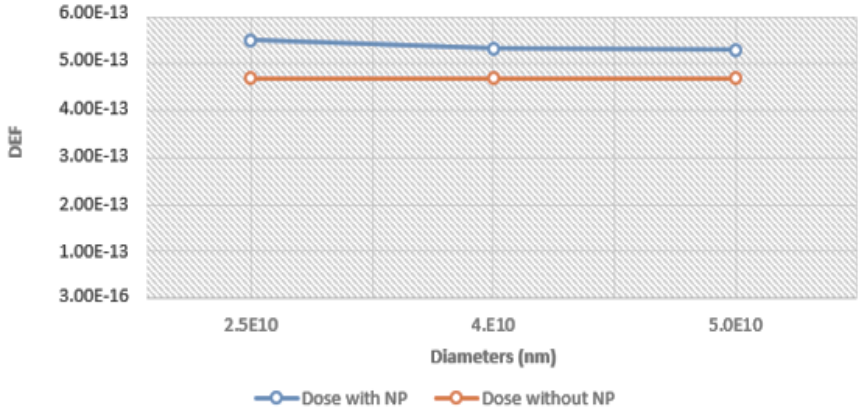


Fig. 11. Bolus absorption dose coefficient (DEF) in the presence of nanoparticles with a concentration of 3% with the energy of 6 MV

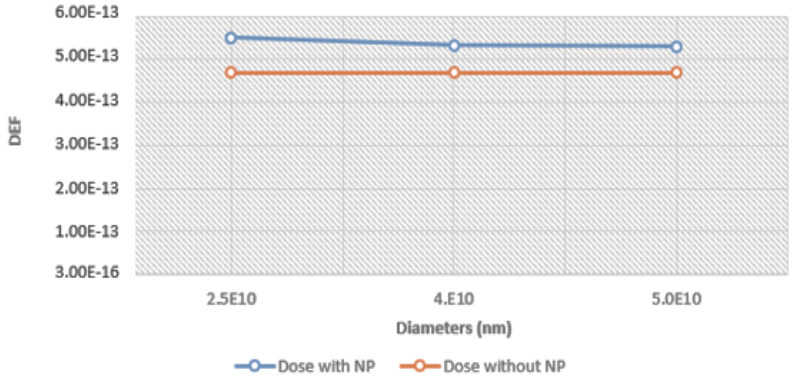


Fig. 12. Comparison of bolus absorption dose (DEF) in the presence of nanoparticles with concentrations of 1 and 3% with 6 MV energy

value of skin surface dose increase coefficient for iron oxide nanoparticles with a concentration of 3% and the dimensions of 25 nm was 1.172.

Experimental study of increasing the skin surface absorption dose (DEF) in the presence of iron oxide nanoparticles (Fe_3o_4) with a concentration of 3% at the energy of MV 6

In this section, the absorbed dose of skin surface in the presence of iron oxide nanoparticles (fe_3o_4) was experimentally investigated and the results were compared with the calculation data of Monte Carlo simulation.

According to the results obtained from the distribution of gold nanoparticles, the highest dose increase was observed in nanoparticles with a radius of 25 nm at a weight concentration of 3%.

This research involved the usage of a bolus with a thickness of 1 cm in the standard dimensions of 10×10 cm^2. To make bolus-containing iron oxide nanoparticles, the weight of ordinary bolus was calculated to be 0.03 and the prepared iron oxide powder nanoparticles in the solvent emulsion of bolus structural materials were combined and molded (Fig. 15).

The advanced Markus phantom and chamber slabs and undoes electrometer were exerted for dosimetry.

As the ordinary bolus and bolus-containing iron

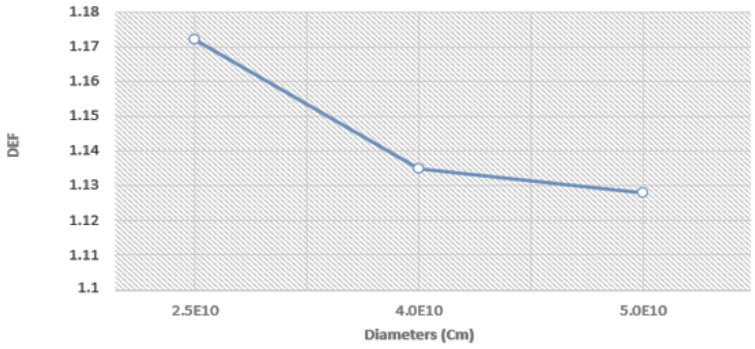


Fig. 13. Absorbed dose of skin surface in the presence and absence of iron oxide nanoparticles with a concentration of 3% at energy of 6 MV

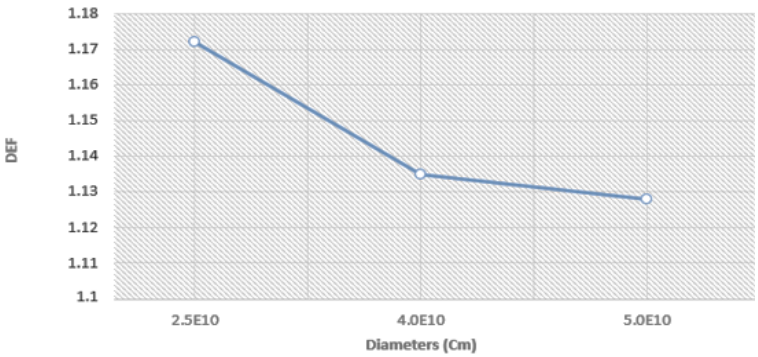


Fig. 14. Increase of absorbed dose of skin surface (DEF) in the presence of iron oxide nanoparticles with a concentration of 3% in 6 MV energy

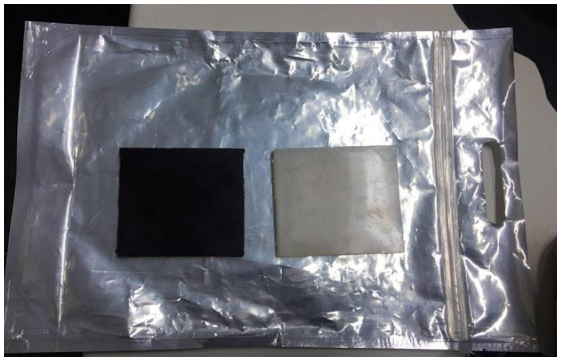


Fig. 15. Right side of ordinary bolus and left side of bolus-containing iron oxide nanoparticles (fe3o4) in the dimensions of cm2 10×10

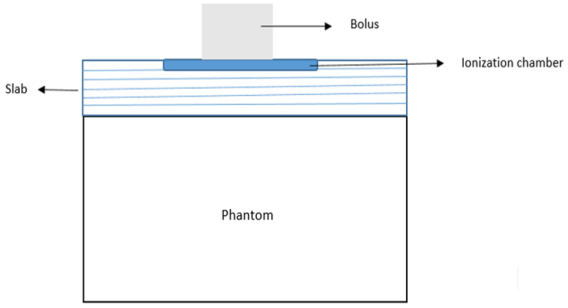
oxide nanoparticles were placed on the chamber, the absorbed dose of Source Surface Distance (SSD) = 100 was obtained on the surface below the chamber.

Marcus chamber is a parallel plate ionization chamber with suitable options for the pre-depth of photon radiation before the depth of build-up and electron radiation. This method was quite fitting for this research since the tissue-equivalent bolus increases the absorbed dose of skin surface and its effectiveness can be observed before the build-up depth.

The absorbed doses of iron oxide nanoparticles with a radius of 25 nm were obtained in accordance to experimental calculations to be 8.1586 E-4 and 9.1784 E-4 in the presence and absence of nanoparticles, respectively. The calculated absorption dose increase factor (DEF) by Equation (2-2) that wad obtained to be 1.124 had a little difference and error when compared to the simulation results.

DISCUSSION

Most of the findings in research in this field have been the result of theoretical work and simulation [16-18]. According to the calculation results of this study in regards to the absorption dose of breast skin, the highest amount of absorption dose increase factor (DEF) was observed at a concentration of 3% by weight and the smaller dimensions of the study (25 nm). The increasing rate of absorption dose (DEF) for gold nanoparticles with a concentration of 1 by Weight percentage and the dimensions of 25 nm was equaled to 1.150, while the dimensions of 40 nm and 50 nm were observed to be 1.133 and 1.129, respectively. The results obtained for gold nanoparticles at a concentration of 3% by weight and for nanoparticles with the dimensions of 25 nm were 1.165, while the dimensions of 40 nm and 50 nm achieved 1.143 and 1.131, which indicates



Fig, 16. Phantom view used in bolus dosimetry in the presence and absence of iron oxide nanoparticles

the occurrence of an increase in the absorbed dose of breast skin surface as a result of enlarging the applied concentration.

According to the results of gold nanoparticles distribution, the highest dose increase in this study was observed from nanoparticles with a radius of 25 nm and a concentration of 3% by weight.

In addition to calculating the dose distribution in breast skin volume through the uniform distribution of gold nanoparticles for evaluating the effectiveness and performing a comparison of the results and experimental data, we also calculated the rate of absorption dose coefficient of skin surface (DEF) in the presence of nanoparticles Iron oxide at a concentration of 3% to compare the results and investigate the obtained data from experimental dosimetry measurements and Monte Carlo simulation calculations.

The increasing rate of Skin surface absorbed dose (DEF) for iron oxide nanoparticles (Fe_3O_4) with the dimensions of 25 nm was 1.172 and for nanoparticles with the dimensions of 40 nm and 50 nm were 1.135 and 1.128, respectively. There was a lack of any evident difference between this observation and the outcomes of Gold nanoparticles, which indicates the effectiveness of nanoparticles in increasing the absorbed dose of skin surface.

In the following, we calculated the experimental dosimetry results from Phantom slab with Marcus dosimeter for iron oxide nanoparticles at an effective concentration of 3% by weight to be 1.124 for nanoparticles with the dimensions of 25 nm. Accordingly, a fine agreement was observed between the results of experimental dosimetry and the calculation of simulations.

According to these outcomes, a general conclusion can be made that points out the effect of exerting gold and iron oxide nanoparticles with

their high atomic number (high Z) on extending the cross-sectional area and increasing the absorbed dose on the skin surface.

The simulation results were indicative of an increase in the absorbed dose of skin surface upon the usage of gold and iron oxide nanoparticles in the bolus, which is in contrast to the cases that lack the existence of nanoparticles. Consequently, the dose increase factor, which is the ratio of the absorbed dose in the presence of nanoparticles to the absorbed dose, increases in the absence of nanoparticles.

CONCLUSION

The presence of nanoparticles in the bolus increases the dose to the skin because when photons collide with the nanoparticles, low-energy Ague electrons are produced and these electrons reach the skin and increase the absorbed dose of the skin. Also in this research energy, the Compton phenomenon dominates and the presence of nanoparticles increases the density of the electrons of the environment, and the probability of Compton increases, and therefore the absorbed dose of the skin surface increases.

Also, when the size of the nanoparticles becomes smaller while the concentration remains constant, it means that the number of nanoparticles increases, and as a result the probability of cross-sectional collision with the nanoparticles increases, and as a result the skin dose increases.

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