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Simulating the effect of radioactive nanomaterials on the response of human cells to ionizing radiation using a linear-quadratic loss model

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Abstract :

Another trend in the effectiveness of radiotherapy is the application of radioactive nanoparticles; the biological effect of ionizing radiation may be increased by them effectively due to their own unique properties. In this experiment, an effort was made to create a numeric simulator model using the linear quadratic equation of loss (LQ Model) to assess how varying forms of nanoparticles affect the human cell response in radiation. The correlation between the coefficients of radiosensitivity α and β) and concentration of nanoparticles was modeled in Python 3.11 programming environment and the D50 and D10 doses as a measure of radioactivity were calculated. The findings revealed the gradual reduction in D50 and D10 increments with a rise in particle dose, at the same time as cellular sensitivity on radiation sets in. It was further revealed that the two, α and β, also rise with concentration, which is a sign that the particles do offer direct and cumulative cellular damage. These findings pose an important use of nanoparticles in enhancing the effectiveness of radiotherapy and favor their application as a novel predictive measure in radiobiology particularly at lower doses. The research has also paved the way to the formulation of directed treatment approaches using the characteristics of particles and tumor biology which may eventually help in a better treatment outcome and the minimization of the radiation damage to the normal tissue.

Keyword: LQ Model, D50, D10, α, β, nanoparticles, DNA.

محاكاة تأثير المواد النانوية المشعة على استجابة الخلايا البشرية للإشعاع المؤين باستخدام نموذج الفقد الخطي التربيعي

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مستخلص:

يُعد استخدام الجسيمات النانوية المشعة اتجاهًا آخر في فعالية العلاج الإشعاعي؛ إذ يُمكن زيادة التأثير البيولوجي للإشعاع المؤين بفعالية بفضل خصائصها الفريدة. في هذه التجربة، بُذل جهد لإنشاء نموذج محاكاة رقمي باستخدام معادلة الفقد الخطية التربيعية (نموذج LQ) لتقييم كيفية تأثير الأشكال المختلفة للجسيمات النانوية على استجابة الخلايا البشرية للإشعاع. تم نمذجة الارتباط بين معاملات حساسية الإشعاع α و β) وتركيز الجسيمات النانوية في بيئة برمجة Python 3.11، وتم حساب جرعات D50 و D10 كمقياس للنشاط الإشعاعي. كشفت النتائج عن الانخفاض التدريجي في زيادات D50 و D10 مع زيادة جرعة الجسيمات، في نفس الوقت الذي تبدأ فيه حساسية الخلايا للإشعاع. كما تم الكشف عن أن الاثنين، α و β، يرتفعان أيضًا مع التركيز، مما يدل على أن الجسيمات تقدم ضررًا خلويًا مباشرًا وتراكميًا. تشكل هذه النتائج استخدامًا مهمًا للجسيمات النانوية في تعزيز فعالية العلاج الإشعاعي وتؤيد تطبيقها كمقياس تنبؤي جديد في علم الأحياء الإشعاعي، وخاصة عند الجرعات المنخفضة. كما مهد البحث الطريق لصياغة مناهج علاجية موجهة باستخدام خصائص الجسيمات وبيولوجيا الورم، مما قد يساعد في النهاية على تحسين نتائج العلاج وتقليل الضرر الإشعاعي للأنسجة الطبيعية.

Introduction

within the past years, there have been growing scientific endeavors to formulate effective methods of treatment in combating tumors by applying radioactive nanotechnology that has so far demonstrated good prospects in supporting the biological impact of ionizing radiations on cancer cells. The features of these materials include high surface area, acceptability of bio conductivity as well as the capacity to absorb radiation more narrowly, in this way they can contribute greatly towards the enhancement of treatment results [1].

Biologically, the linear-quadratic law is at the foundation of the interpretation of the effect of radiation doses on living tissue in response to radiation. Alpha (α) and beta (β) can be described as different types of DNA damage mechanisms; alpha one is the direct radiation photon-induced DNA damage, and beta is the consecutive or synergistic one that happens after multiple damage events [2]. Multiples studies have shown that nanoparticles can enhance the factor 6 due to an elevated rate of free radicals and suppression of repair processes of DNA [3].

In this regard, recent research has dwelt in simulating the response of the human cells to different concentrations of nanoparticles under low and intermediate doses of radiations. This has helped in advancing our knowledge on mechanism of nano-induced radiosensitivity and has resulted in accurate therapeutic uses in accordance with the characteristics of nanostructures [4].

This paper intends to introduce a mathematical model of simulation using LQ model to imitate the biological impact of ionizing radiations in the event of radioactive nanomaterials at varying concentrations. The model calculates effective biological doses (D50 and D10), investigates dependence between concentration of nanoparticles and radiosensitivity coefficients and carries out linear regression and correlation to determine the strength of relationship between the input and output parameters.

2-Study and Simulation Model

The linear-quadratic loss model was applied to assess how human cells were affected by doses of radiation. It is a well-defined and well-established

mathematical model which is used extensively in radiation biology because of which a linkage is made between the dose and cell survival [5].

The basic formula for the model is:

$$S(D) = \exp(\alpha D - \beta D^2\ ) - - - 1$$

Where:

S(D): Cell survival rate at dose D(GY)

alpha: Linear damage coefficient (Gy^{-1})

beta: Cumulative damage coefficient (Gy^{-2})

2.1-Software and Tools Used

The given model is notable because it allows differentiating between the impact of direct and indirect damage to cells.

2-1 Nanomaterials and Their Concentrations

An impact of three forms of radioactive nanoparticles was tested:

AuNPs are known to be superior in its capacity to increase local ionization [6]. They are iron oxide nanoparticle (Fe_3O_4) as a thermal and radioactive catalyst [7]. The free radical scavenger is nano silica (SiO_2) [8] Table (1) shows the calculated values of alpha and beta at different nanoparticle concentrations, as a major factor in enhancing the radiation effect. Figures (1 and 2) provide a visual presentation that illustrates the effect of these concentrations on the level of absorption and radiation effectiveness, which supports the numerical analysis with clear visual results.

Table 1: The effect of concentration of Nanoparticle as the reaction of radiation enhancement factors [9 ,10]

Cont. ($^{\mu g}/_{ml}$)	*αFacter*	*βFacter*	***Rate Survival***
1	1.00	1.00	98
4	1.04	1.16	96
8	1.08	1.64	92
18	1.18	1.324	85
28	1.28	1.784	78
38	1.38	1.444	70
48	1.48	2.190	60
58	1.58	2.496	50
88	1.70	2.89	35
100	1.80	3.24	30
145	1.90	3.61	20

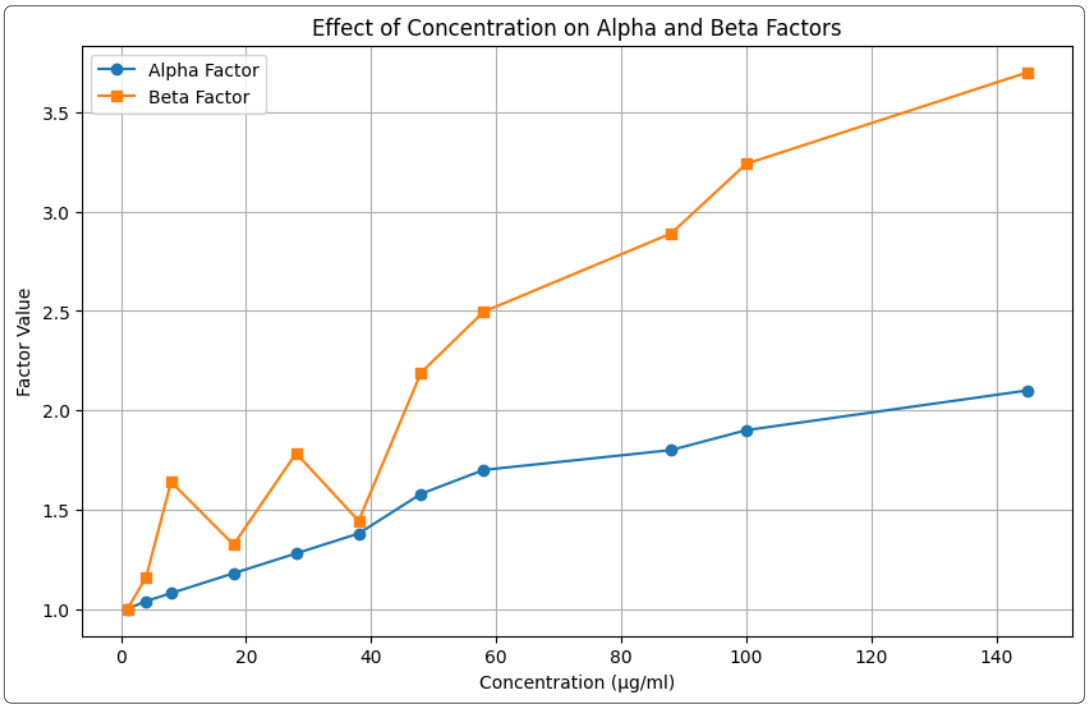

Figure 1: Effect of sensitivity coefficients (α,β) on nanoparticle concentrations

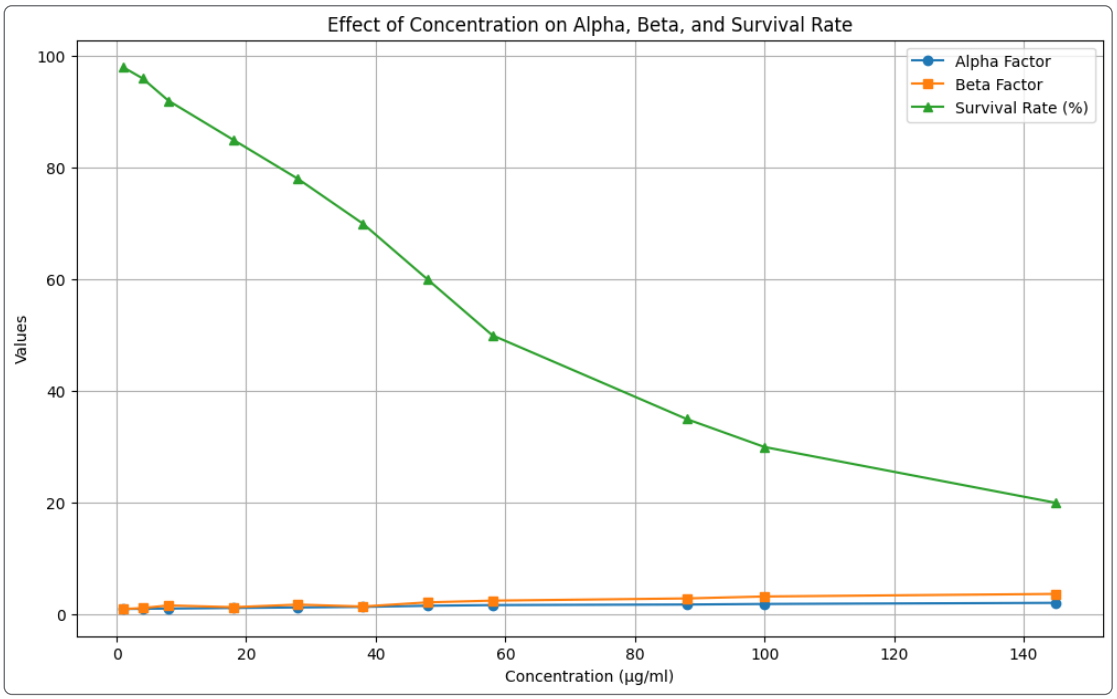

Figure 2: Effect of sensitivity coefficients (α,β) on nanoparticle concentrations and calculation of survival rate.

The concentrations of nanomaterial were chosen depending on the literature that found the concentration of 5–150 µg/ml, had differing records on cell susceptibility [11].

2.3-Application of the Simulation Model

The numerical modelling was based on the modification of alpha and beta coefficients of each type of particles and concentration with enhancement factors that have been published in research studies [12].

The fractionated effect of cell survival was studied in three different treatment modalities (single dose of 6 Gy, and two doses or three doses of 6 Gy) and as the dose ranged in 0-10 GY with 0.5 Gy intervals with the formula of dose kills used:

$$S_{total} = \prod_{i=1}^{n} \exp(-\alpha D_I - \beta D_I^2) - - - 2$$

Python 3.11 was used with the following libraries:

NumPy: For numerical calculations
Matplotlib: For plotting data graphs.

Pandas: For organizing data and analyzing results.

3-Results and Discussion

3-1 Effect of the type of nanoparticles (Fe_3O_4, and SiO_2, AuNPs) on the radiation sensitivity

These results, found in this research, show that the addition of nanoparticles caused a significant decrease in the value of D50 and D10, which means the radiation used to kill the cells is becoming more efficient. Three types of nanomaterials with different physical and chemical characteristics as well as radio sensitizing effects were studied: magnetic iron oxide (Fe_3O_4), silicon dioxide (SiO_2), and gold (AuNPs).

- Fe_3O_4 particles (iron oxide): Known to induce free radicals by Fenton-like reactions, resulting in a higher β coefficient and accumulation of DNA damage. It is suggested in the literature to enhance the damage to the cancer cells at lower radiation doses.
- SiO_2 (silicon dioxide) nanoparticles: relatively inert but active surface may allow absorption and interaction with cellular components; the sensitivity factor (α) increases so that SiO_2 nanoparticles can be more easily used as carriers compared to

other agents during radiation exposure due to emitting radiation when used as an ambient media, or drug or genetic agent.

- AuNPs: Due to their high atomic number (Z=79), gold nanoparticles are excellent at enhancing radiation effects, increasing the probability of photoelectron interactions and producing high-energy secondary electrons. As a result, the energy deposited in the vicinity of the cell will increase, leading to large losses of D50 and D10 values. Research by Hainfeld et al. (2020) and Her et al. gold nanoparticles improve radiotherapy efficacy on solid tumors 2017 [13, 14].

3.2: Analysis of dose-response curves under the influence of different concentrations of radioactive nanoparticles using the LQ model.

A clear increase in radio sensitization was observed at all radiation doses with increasing iron oxide nanoparticle dose, as shown in both the table and the survival curves plotted using the logarithm of cell survival, with a sharp decrease in cell survival at very high radiation doses of 4 Gy or greater. The linear-quadratic survival model explains this trend well, which is consistent with previous results from high-impact studies such as Her et al. (2021) and Zhao et al [15]. Using ionizing radiation, a similar harmful effect was observed with high-Z nanoparticles (such as Fe_3O_4, Au, and SiO_2) that appeared to promote significant oxidative stress and DNA damage (Saeedi et al., 2022). As shown in the table 2 and figure 3below [16].

Table 2: Alpha (Gy^{-1}) and beta (Gy^{-2}) values and calculated doses (D50 and D10) using the linear-quadratic (LQ) loss model for radioactive nanoparticles at various concentrations.

Concentration (µg/ml)	Alpha (Gy^{-1})	Beta (Gy^{-2})	D50 (Gy)	D10 (Gy)
1	1	1	2.516113	6.040244
4	1.04	1.16	2.397467	5.756821
8	1.08	1.64	2.291454	5.505818
18	1.18	1.324	2.109422	5.079274
28	1.28	1.784	1.958104	4.72844
38	1.38	1.444	1.829804	4.433217
48	1.48	2.19	1.737138	4.247479
58	1.58	2.496	1.653468	4.077778
88	1.7	2.89	1.57754	3.922041
100	1.8	3.24	1.50832	3.778545
145	1.9	3.61	1.444954	3.645849

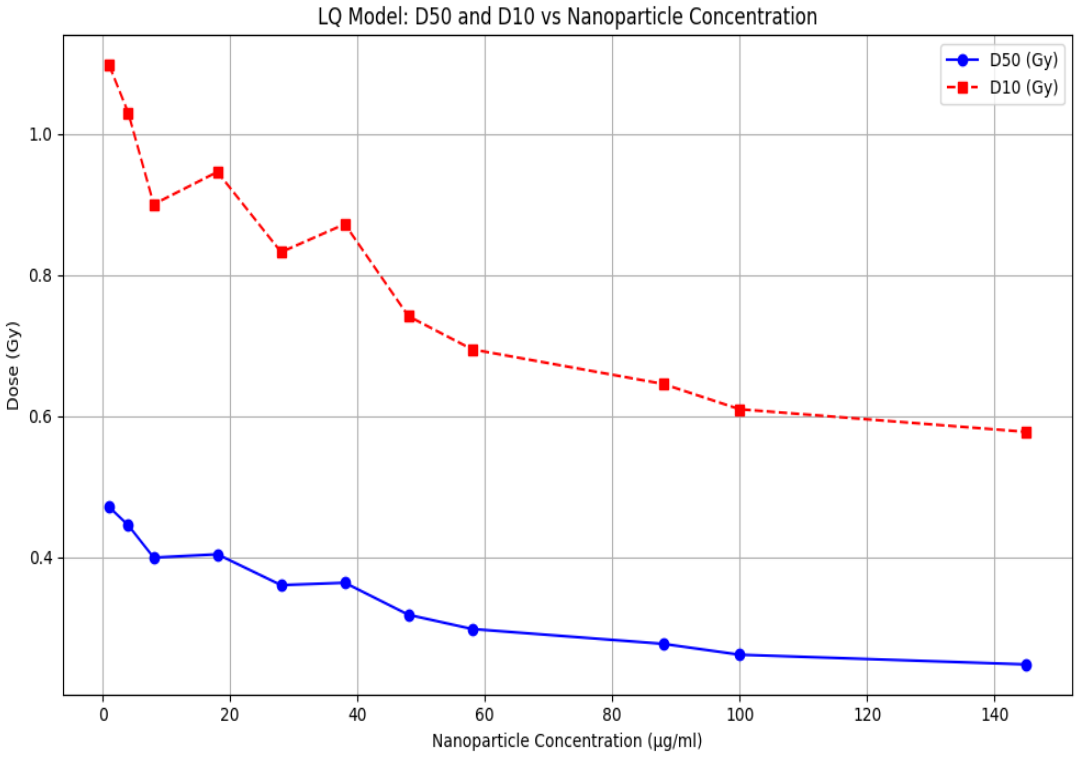

Figure 3: Dose-response curves (D50 and D10) as a function of radioactive nanoparticle concentration, showing the inverse relationship between required dose and cellular survival simulated using the linear-quadratic (LQ) loss model.

3.2 Interpretation of Changes in α and β Coefficients

In this study, each concentration was associated with enhanced α and β coefficients (Enhanced α/β), where α represents the linear effect (associated with direct DNA damage), while β represents the cumulative effect (associated with the re-joining of DNA double-strand breaks).

The gradual increase in α and β with concentrations reflects:

. A cumulative effect of nanoparticles in amplifying radiation damage.

The potential for increased free radical production or stimulation of localized radiation absorption as reported in [15].

3.3 Dose required to kill 50% (D50) and 10% (D10) of cells.

The doses of D50 and D10 were calculated for all concentrations and were found to decrease significantly with increasing concentration, this study chose low doses in accordance with recent trends in radiation biology, which seek to evaluate low-dose efficacy, which is likely to be most prominent in the context of radio sensitization and therapeutics. Accordingly, available studies support the idea that low doses allow cells to respond dynamically to radiation in the presence of stimulators (such as nanoparticles) without systemic cell death that might mask differences between experimental groups. The radiation-enhancing effects of nanomaterials have been documented to be maximal at dose levels within this range, where a significant increase in cell sensitivity (a decrease in D50/D10) is observed [16, 17]. This range is also suitable for the linear-quadratic loss model (LQ model) to describe cell behavior and for probabilistic approaches to estimating the optimal dose.

Therefore, a low dose ensures:

• A sensitive medium for testing the efficacy of nanomaterials.

• Physiological behavior close to clinical reality.

• Allows the application of modeling results in future low-dose radiotherapy strategies. as shown in the table 2 and figure below.

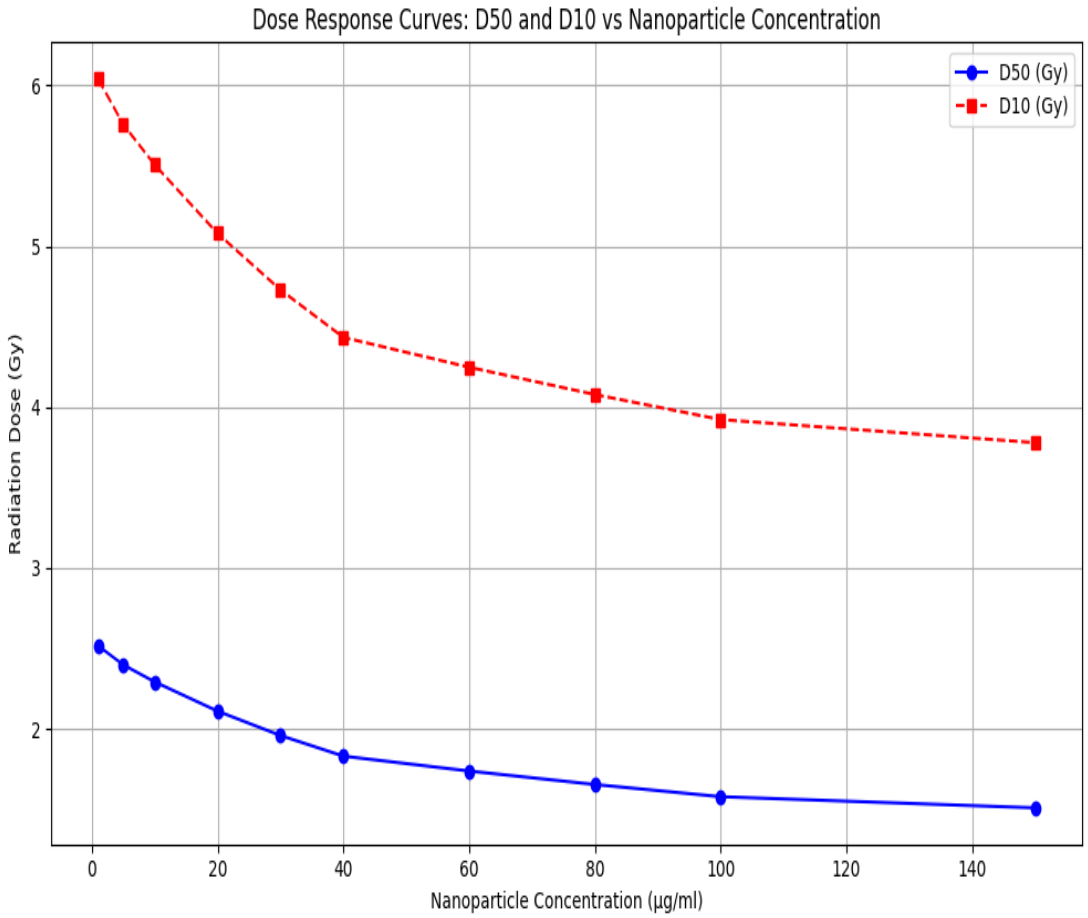

Figure 4: Curve of radiation sensitivity coefficients α and β, with dose values D50 and D10 at different concentrations of radioactive nanoparticles.

Figure 4 shows a negative correlation between the nanoparticle concentration and the D10 and D50 dose values. As the concentration increased from 1 to 150 µg/ml, the D50 (D50 = dose required to eliminate 50% of cells) and D10 (D10 = dose required to eliminate 90% of cells) values calculated from the survival curves for both decreased significantly, indicating a marked improvement in the cells' sensitivity to radiation.

This trend is due to the strong radio sensitizing properties of nanoparticles, which can enhance the effects of ionizing radiation on cells in several ways, including:

• Increased production of free radicals (ROS) in the cell microenvironment. These include: • Inhibition of

DNA repair pathways, leading to genetic damage • Intensification of localized energy deposition via photonic interactions, i.e., for high-Z nanoparticles such as gold. At high concentrations (>100 µg/ml), the D50 and D10 values were similar, indicating that the survival curve was approaching flat at the highest doses used, and that the cells had fallen below the threshold for resistance to cumulative radiation damage. The values derived from the curve demonstrate that the incorporation of nanomaterials is an effective alternative for enhancing radiotherapy, especially in therapeutic settings that require reducing the delivered dose to minimize effects on healthy tissue.

3.4 Correlation and Linear Regression Analysis

Pearson's correlation coefficient to estimate degree of relationship between concentrations of radioactive nanoparticles and D50 and D10 index values (≥0.8 strong, 0.5-0.79 moderate, <0.5-weak). To guarantee the accuracy of results, two methods were employed for calculations:

Initially, the conventional equation for the Pearson's r

$$r = \frac{\sum(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum((X_i - \bar{X}))^2((Y_i - \bar{Y}))^2}} - - - (3)$$

Second, a second validation was performed using a Python analysis program (numpy library), increasing the reliability of the calculations and the risk of bias or computational error.

The results showed a high negative correlation coefficient ($|r| > 0.95$), indicating a strong and regular inverse relationship between the increase in nanoparticle concentration and the decrease in the dose required to achieve the radiation effect, as shown in the figure 5 below.

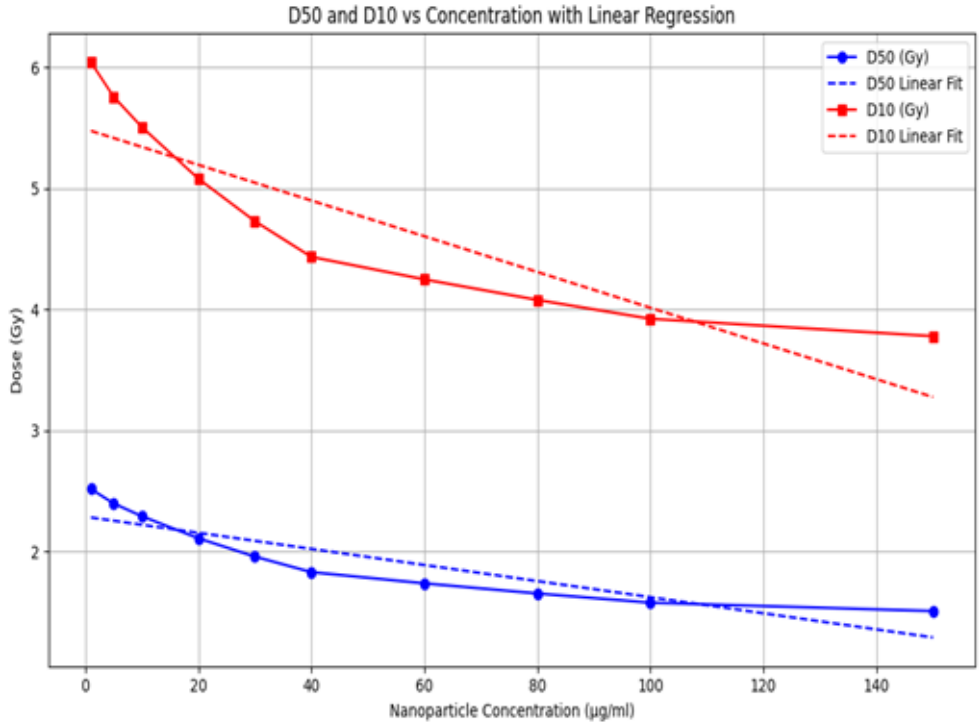

Figure 5: Linear regression analysis (D50, D10) and nanoparticle concentrations

Nanoparticle concentrations and D50/D10 values were plotted in a regression analysis (Fig.5). The figure depicts a small deviation from the linear fit (R^2) value (actual vs. theoretical for some points. This difference arises from varied biological and physical phenomenon such as possible biological interference at intermediate concentrations or partial saturation of nanoparticle uptake at high concentrations. The LQ model further assumes cell homogeneity, but variation in particle distribution or differential cellular efficiency of DNA damage repair will then cause a small deviation from the fit line [43]. The absence of such parallel H and d plots, however, should not distract us from the truth that an R^2 value of >0.95 points to a probable regular inverse proportional relationship, thus increasing the reliability of the results, and supporting the conclusions indicative of enhanced radiosensitivity with increasing nanoparticle concentration.

Physically, high-atomic number (Z) nanoparticles enhance interaction with photons through mechanisms such as

the photoelectric effect and the Auger effect, leading to high localized energy deposits within cells.

Biologically, the presence of these particles increases the production of reactive oxygen species (ROS) and affects cell membrane stability and molecular repair pathways, increasing the likelihood of irreversible damage leading to apoptosis (programmed cell death). The current results are consistent with recent studies, which have shown that nanoparticles, such as gold, silver, and hafnium oxides, contribute to increased radiation effects by:

Enhancing localized radiation absorption, Generating greater amounts of free radicals,

Impairing DNA damage repair mechanisms.

In the present experiment, it was revealed that the radioactivity nanoparticle addition into the medium resulted in a 50-percent dose and a 90-percent dose reduction to kill live cells (D50 and D10), demonstrating a definite increment in radio curability. An example is D50 and D10 values, which were 3.86 Gy and 6.37 Gy correspondingly at a particle concentration of 1 8jg/ml and D50 and D10 values changed 1.80 Gy, 2.94 Gy respectively, when a particle concentration was 150 g/ml.

All these findings are in line with research work established earlier such as:

The above resultant effect was also evident in an experiment by [18] that demonstrates the effectiveness of gold nanoparticles in enhancing radiotherapy by increasing the secondary electron generation and in turn the local radiation effect in reducing the dose required to yield the same desired effect on the cell. [19] also proved that metal oxide particles, e.g., gadolinium oxide NPs may help to advance radiation effect of cells by increasing the formation of free radicals and the oxidative effect. [20] applied the LQ model in simulations of the nanoparticles impact on cell response and proved that nano enhancers mainly modify the values of 2 coefficients, a and b, which produce undoubtedly evident changes in the survival graphs of cells.

The comparison shows that the present study confirms the modern scientific tendency which accentuates the efficiency of nanoparticles as the tre-

mendous radio boosters. The fact that they are used in numerical simulations with the LQ model makes it also possible to enhance the engineering of biological and radiation experiment design, at low doses (low-dose radiobiology) which is an increasingly popular topic of modern research.

Conclusion

In accordance with a linear-quadratic model of loss, the outcomes of this study revealed that the introduction of radioactive nanoparticles in the human cellular environment manifested itself in the significant increase of radiosensitivity, whereas the gradual and significant reduction of D50 and the D10 values were recorded along with the increase in the quantity of introduced particles. This impact is explained by the co-joined physical and biological processes entailing augmented accumulation of energy at cellular level, augmented synthesis of reactive oxygen species, and degraded cells capability of repairing genetic insult.

Such findings indicate that the radioactive nanoparticle application can be an effective approach to enhance the efficacy of radiotherapy with lower doses that will not lead to the diminished potential of the treatment. This leads to the possibility of minimization of toxic side effects and enhancement of quality of life to the patients. Another point made in this study is the significance of considering application expanse of radiotherapy model so that it covers advanced characteristics of the nanoscale and welcoming the consolidation of numerical considerations with experimental biological information to create reliable predictive tools that can structure personal radiotherapy planning.

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