

Radiation Physics and Engineering 2027; ?(?):?–?

Monte Carlo simulation of the effects of high-Z elemental impurities on proton therapy dose distribution

Behshad Valizadeh^a, Elham Saniei^b, Armin Mosayebi^a, Seyed Pezhman Shirmardi^{a,*},
Hamideh Daneshvar^a, Babak Sepehri^b

^aRadiation Processing and Dosimetry Research Group, Radiation Application Research Institute, Nuclear Science and Technology Research Institute, Tehran, Iran

^bDepartment of Medical Radiation Engineering, CT. C., Islamic Azad University, Tehran, Iran

HIGHLIGHTS

-
-
-
-

ABSTRACT

Proton therapy utilizes the Bragg peak to deliver highly localized radiation doses while minimizing exposure to surrounding healthy tissues. However, tissue heterogeneities and the presence of high-atomic-number (high-Z) impurities may alter proton transport and dose deposition. In this study, Monte Carlo simulations using the MCNPX code were performed to investigate the effects of proton beam parameters, tissue heterogeneities, and high-Z impurities on proton dose distributions and Bragg peak characteristics. The influence of proton energy, beam radius, heterogeneity position, and embedded gold, lead, and uranium impurities was evaluated through analyses of penetration depth, deposited energy, and depth-dose profiles. The results showed that increasing proton energy enhanced penetration depth while reducing the maximum deposited energy, whereas beam radius mainly affected peak intensity. Tissue heterogeneities produced noticeable shifts and distortions in Bragg peak profiles depending on their density and location. Furthermore, the introduction of high-Z impurities reduced proton penetration depth from 5.07 cm to 5.01-5.03 cm and decreased deposited energy from 1.64 to 1.59-1.61 MeV.cm⁻³. These findings demonstrate that both tissue heterogeneities and trace high-Z impurities can significantly modify proton beam behavior and dose distributions. Accurate modeling of such effects is therefore essential for improving dosimetric accuracy and optimizing proton therapy treatment planning.

KEYWORDS

Proton therapy
Dose Distribution
Monte Carlo Simulation
High-Z Materials
Impurities
Bragg Peak

HISTORY

Received:
Revised:
Accepted:
Published:

1 Introduction

Proton therapy offers a significant advantage over conventional photon radiotherapy due to the unique physical characteristics of protons, particularly the presence of the Bragg peak in their depth-dose distribution. As protons penetrate matter, they gradually lose their kinetic energy and deposit a large fraction of their energy near the end of their range before coming to a complete stop. This behavior results in a substantial reduction in the dose

delivered to surrounding healthy tissues compared with photon beams, therefore providing the potential for an improved therapeutic ratio (Lane et al., 2023; Newhauser and Zhang, 2015). The primary objective of radiotherapy is to deliver the maximum possible dose to the tumor volume while minimizing radiation exposure to adjacent normal tissues and organs. Currently, a large proportion of clinical radiotherapy applications are based on MV photon beams. In photon radiotherapy, although the initial dose buildup region provides an increase in dose deposi-

*Corresponding author: p.shirmardi@aut.ac.ir

tion at shallow depths, photons continue to deposit energy along their entire path due to attenuation and scattering processes within the tissue. Therefore, multiple irradiation fields from different angles are commonly employed to achieve adequate tumor coverage while limiting the dose received by healthy tissues. In contrast, protons, owing to their increased energy loss rate with decreasing velocity and their finite range in matter, are capable of depositing radiation dose more precisely within the target region (Durante and Loeffler, 2010). Therapeutic proton beams typically have energies in the range of 70–250 MeV and continuously lose energy as they travel through matter. The increase in linear energy transfer (LET) with decreasing proton velocity leads to enhanced energy deposition near the end of the particle trajectory (Paganetti, 2025). This process results in a distinct maximum in the depth-dose distribution, known as the Bragg peak. The depth of the Bragg peak, or proton range, depends on the initial proton energy and the physical characteristics of the traversed medium. Beyond this region, the dose rapidly decreases as protons lose their remaining energy and stop. Although lateral scattering occurs during proton transport through matter, the dose outside the primary beam path remains considerably lower compared with photon irradiation (Ekinici and Bölükdemir, 2019). Therapeutic proton beams are generated using accelerators such as cyclotrons and synchrotrons. The concept of using protons for cancer treatment was first proposed by Wilson in 1946, and in subsequent decades, with advances in accelerator technology and the development of dedicated medical systems, proton therapy gradually transitioned from research facilities to clinical applications (Vestergaard et al., 2023). Despite the considerable advantages of proton therapy, accurate prediction of proton range and precise calculation of dose distribution in realistic human tissues remain major challenges. Proton dose deposition is highly sensitive to small variations in elemental composition, density, and anatomical heterogeneities within the irradiated medium. Consequently, inaccurate modeling of tissue physical properties may lead to shifts in the Bragg peak position and difference between the calculated and actual dose delivered to the patient (Chao et al., 2017; Cheung et al., 2009). In recent years, various approaches have been developed to improve dose calculation accuracy and proton range prediction. Among these methods, Monte Carlo simulation has attracted significant attention as one of the most accurate techniques for modeling particle transport in matter (Jabbari, 2011). By statistically simulating the trajectories of a large number of particles and incorporating various physical interactions, including multiple scattering, elastic collisions, nuclear interactions, and energy transfer processes, Monte Carlo methods enable detailed evaluation of proton behavior and dose variations in complex and heterogeneous environments (Baumann et al., 2023; Holmes et al., 2024). Therefore, accurate patient-specific tissue modeling has become an essential component of modern treatment planning systems (Vestergaard et al., 2023). This issue becomes particularly important when the proton beam path includes materials with elemental compositions different from those of reference tissues. The

human body is not a completely homogeneous medium, and structures such as bone, teeth, metallic implants, contrast agents, and local variations in tissue composition can influence proton-matter interactions. Changes in electron density and stopping power may alter proton range, shift the Bragg peak position, modify the depth-dose profile, and ultimately reduce the accuracy of dose delivery to the target volume. This concern is especially relevant for tumors located near sensitive anatomical structures or along the direct path of the proton beam (Pettersson et al., 2024). One of the less extensively investigated factors in this context is the presence of elemental impurities or high-Z materials within the proton transport medium. Although the effects of density heterogeneities and variations among major biological tissues have been widely investigated, the systematic influence of heavy elements with different elemental compositions on proton beam behavior remains insufficiently explored (Cohilis et al., 2023). Due to their distinct physical interaction characteristics, high-Z elements may affect energy transfer mechanisms, scattering processes, and proton stopping behavior (Jia et al., 2015). The presence of materials such as gold, lead, and other high-Z elements may modify the deposited energy, proton penetration depth, and the dose fall-off slope beyond the Bragg peak. Although elements such as uranium are not commonly present under clinical conditions, their investigation as an extremely high-Z material provides valuable insight into the limiting behavior of high-Z inclusions and the sensitivity of proton dose distributions to substantial changes in elemental composition (Tabbakh, 2026). Therefore, investigating the effects of impurities and high-Z elements on proton dose distribution can provide valuable information for improving treatment planning accuracy, reducing computational uncertainties, and developing more realistic models of human tissues (Vestergaard et al., 2023).

The aim of this study is to evaluate the influence of metallic impurities, including gold, lead, and uranium, on proton beam dose distribution using Monte Carlo simulations. Specifically, the effects of these impurities on key proton beam parameters, including deposited energy, penetration depth, and dose fall-off slope, are investigated in a tissue-equivalent medium. The findings of this study may contribute to a better understanding of the impact of elemental heterogeneities on proton transport and highlight the importance of considering high-Z materials in proton therapy dosimetric calculations.

2 Materials and Methods

2.1 Monte Carlo Simulation Setup

The MCNPX code (version 2.6.0) was used to simulate proton transport and radiation interactions within the phantom and to calculate the resulting energy deposition and dose distributions. MCNPX is a general-purpose Monte Carlo radiation transport code that enables the simulation of particle transport in complex three-dimensional geometries. In the present study, the simulation input was defined using appropriate source, geometry,

material, physics, and tally cards according to the requirements of the proton therapy model. Proton transport was modeled using the physics models implemented in MCNPX and the available nuclear cross-section libraries. The PAR=9 option was used to define proton transport, and the PHYS card was applied for variance reduction. An energy cutoff of 0.001 MeV (1 keV) and particle histories were used for each simulation. The proton beam was modeled using a directional plane source in vacuum. The source was positioned 10 cm upstream of the phantom entrance, with the initial proton direction parallel to the beam axis. A circular source cross-section with a radius of 1 cm and a uniform spatial distribution was defined. The reference water phantom had dimensions of cm^3 with a cm^2 field size and was divided into 1-mm cubic voxels using a T-MESH card. Phantom materials were selected according to National Institute of Standards and Technology (NIST) data. Water was used as the primary material, while bone and adipose tissue were incorporated as heterogeneous materials, with densities of 1.85 and 0.92 g.cm^{-3} , respectively. For the high-Z impurity simulations, a 7-cm-thick adipose phantom with a density of 0.9869 g.cm^{-3} was divided into layers of 4.5, 1.0, and 1.5 cm. The central 1-cm layer was separately doped with Au, Pb, and U at 100 ppm using an 80 MeV proton beam. The F6 tally was used to calculate the energy deposition and dose distribution in the regions of interest. The T-MESH card was used to evaluate the spatial distribution of the deposited energy within the cubic voxels. Proton energies ranging from 10 to 100 MeV were investigated. The Spread-Out Bragg Peak (SOBP) was constructed by combining Bragg curves at 40, 44, 47, 50, 53, 56, 59, and 62 MeV using optimized weighting factors. The effects of tissue heterogeneity were evaluated using bone and adipose layers with thicknesses of 0.1, 0.5, and 1.0 cm.

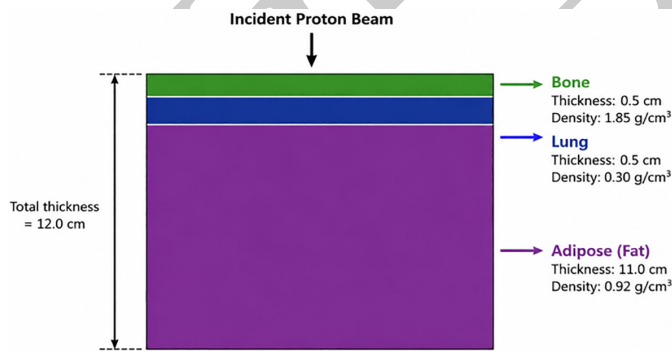


Figure 1: Simulated geometry consisting of a heterogeneous phantom composed of bone, lung, and adipose tissues.

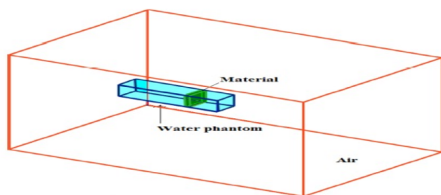


Figure 2: Water phantom with heterogeneous materials arrangement.

2.2 Impact of Tissue Impurities on the Bragg Curve

In this study, a phantom consisting of adipose tissue with a thickness of 7 cm and a density of 0.9869 g.cm^{-3} was designed. The adipose tissue phantom was divided into three layers with thicknesses of 4.5 cm, 1 cm, and 1.5 cm. To investigate the effect of tissue impurities, a 1 cm-thick layer was separately doped with gold (Au), lead (Pb), and uranium (U) at a concentration of 100 ppm. The proton beam energy was set to 80 MeV for all simulations. To reduce statistical uncertainty, the PHYS card was used for variance reduction, and the absorbed dose in the region of interest was calculated using the F6 tally and a cubic T-MESH card.

2.3 Monte Carlo Investigation of Spread-Out Bragg Peak (SOBP) Formation

The Spread-Out Bragg Peak (SOBP) was generated by superimposing proton beams of different energies using appropriate weighting factors. Two independent simulation approaches were employed to evaluate SOBP formation. In the first approach, monoenergetic proton simulations were performed to analyze beam behavior in a heterogeneous layered phantom composed of bone, lung, and adipose tissues with a total thickness of 12 cm. Proton energies ranging from 10 to 100 MeV, with 10 MeV increments, were considered. For each energy, the associated Bragg curves and depth-dose profiles were extracted to assess the feasibility of constructing an SOBP through linear superposition. The F6 tally was used to calculate the absorbed dose and energy deposition within the region of interest, while a cubic T-MESH card was used to evaluate their spatial distribution. The simulation geometry consisted of a stratified arrangement of bone, lung, and fat layers with defined thicknesses to represent a realistic heterogeneous phantom for proton transport analysis (Fig. 1). This configuration enabled the investigation of energy-dependent penetration depth and dose modulation in layered biological media. In the second method, the SOBP was constructed by superimposing individual monoenergetic proton Bragg curves obtained from separate MCNPX simulations. Proton energies ranging from 40 to 62 MeV (40, 44, 47, 50, 53, 56, 59, and 62 MeV) were selected to cover the desired target region. The contribution of each energy component was adjusted using optimized weighting factors to achieve a uniform dose plateau. The final SOBP distribution was obtained by linear combination of the weighted dose profiles, and the F6 tally was used to calculate the energy deposition in each cell of the phantom.

2.4 Dose Distribution and Bragg Peak Variations in Heterogeneous Tissues

In this section, the influence of heterogeneous material type and placement on Bragg peak behavior was investigated. The study was performed under three distinct scenarios. In the first scenario, a 12-cm-thick water phantom was irradiated using a 108.8 MeV proton beam, serving

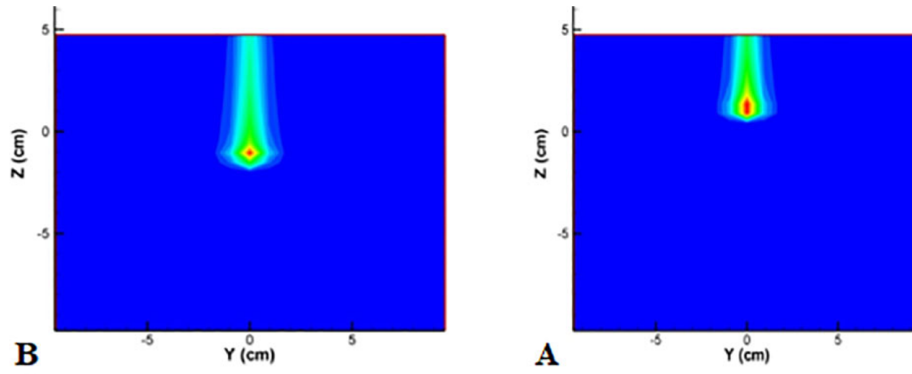


Figure 3: Proton beam penetration for (a) 70 MeV and (b) 90 MeV with a constant source radius of 1 (cm).

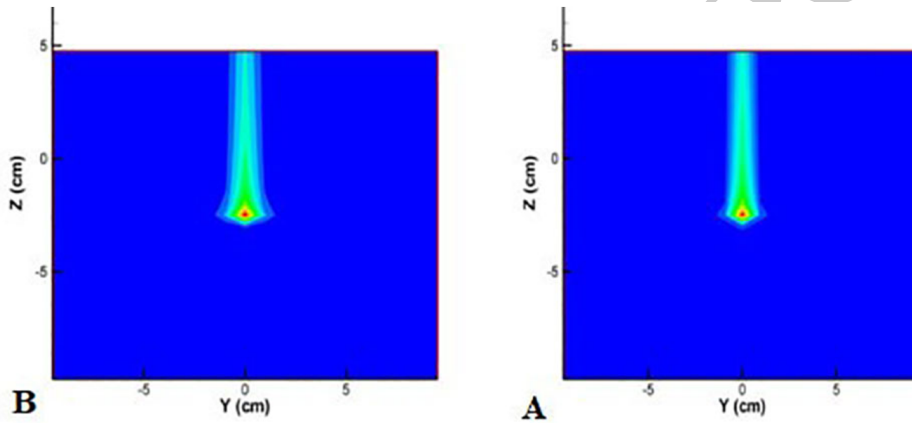


Figure 4: Proton beam dose distribution for (a) 0.7 cm source radius and (b) 0.9 cm source radius at a constant energy of 100 (MeV).

as the reference case. The resulting depth-dose distribution and Bragg curve were obtained, and the position of maximum energy deposition was identified as the Bragg peak. This depth was subsequently used as a reference for positioning heterogeneous materials in the following scenarios. In the second scenario, the effect of introducing heterogeneous materials at the Bragg peak region was examined. Fat and dense bone were separately inserted at this depth with thicknesses of 0.1, 0.5, and 1 cm. The resulting variations in Bragg peak position, shape, and magnitude were analyzed for each material and thickness. In the third scenario, the same heterogeneous materials and thicknesses were introduced in the plateau region of the Bragg curve to evaluate their effect outside the peak region. The associated changes in dose distribution and Bragg peak characteristics were systematically assessed. As shown in Fig. 2, a schematic representation of the water phantom and the configuration of heterogeneous inserts is presented. The setup includes layers of fat and dense bone embedded within a surrounding air environment, and was used to investigate their impact on proton dose deposition and Bragg peak behavior.

3 Results and discussion

In this study, the effects of proton source energy and source radius on penetration characteristics and dose dis-

tribution were investigated under two separate conditions. In the first case, a water phantom with a fixed source radius was simulated to evaluate the influence of varying proton beam energy on penetration depth. The resulting dose distributions for different energies were extracted, and two-dimensional penetration maps were generated using Tecplot software. The results are presented in Fig. 3. As shown, increasing proton energy leads to a deeper penetration along the Z-axis and an associated shift of the Bragg peak region toward greater depths, while the lateral dose profile remains largely unchanged. In the second case, the proton beam energy was kept constant, and the effect of varying source radius was analyzed. For different source radii, simulation outputs were processed and two-dimensional dose distributions were again visualized using Tecplot, as shown in Fig. 4. The results indicate that increasing the source radius leads to enhanced lateral beam spreading along the Y-axis and a broader dose distribution. However, the depth of maximum dose deposition remains nearly unchanged, suggesting that penetration depth is primarily governed by proton beam energy rather than source radius.

3.1 Energy-Dependent Proton Transport in Homogeneous and Heterogeneous Tissues

In this section, the influence of tissue type and environmental heterogeneity on proton beam penetration depth

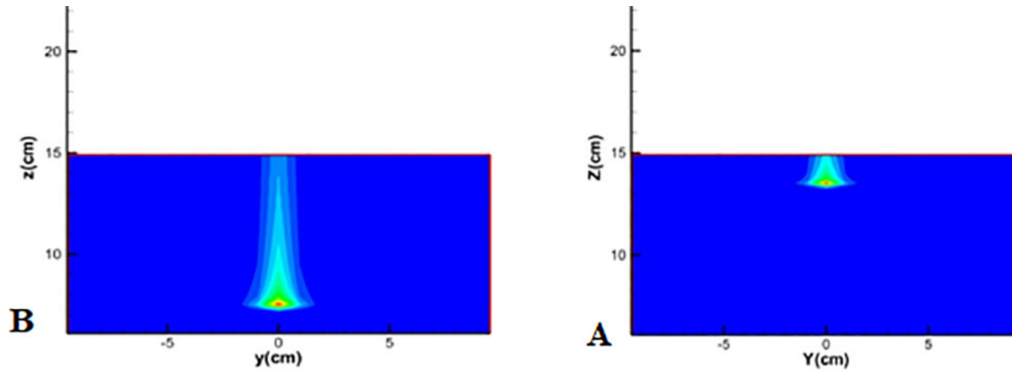


Figure 5: Proton beam penetration in (a) bone tissue and (b) lung tissue at 50 (MeV) (9 cm thickness).

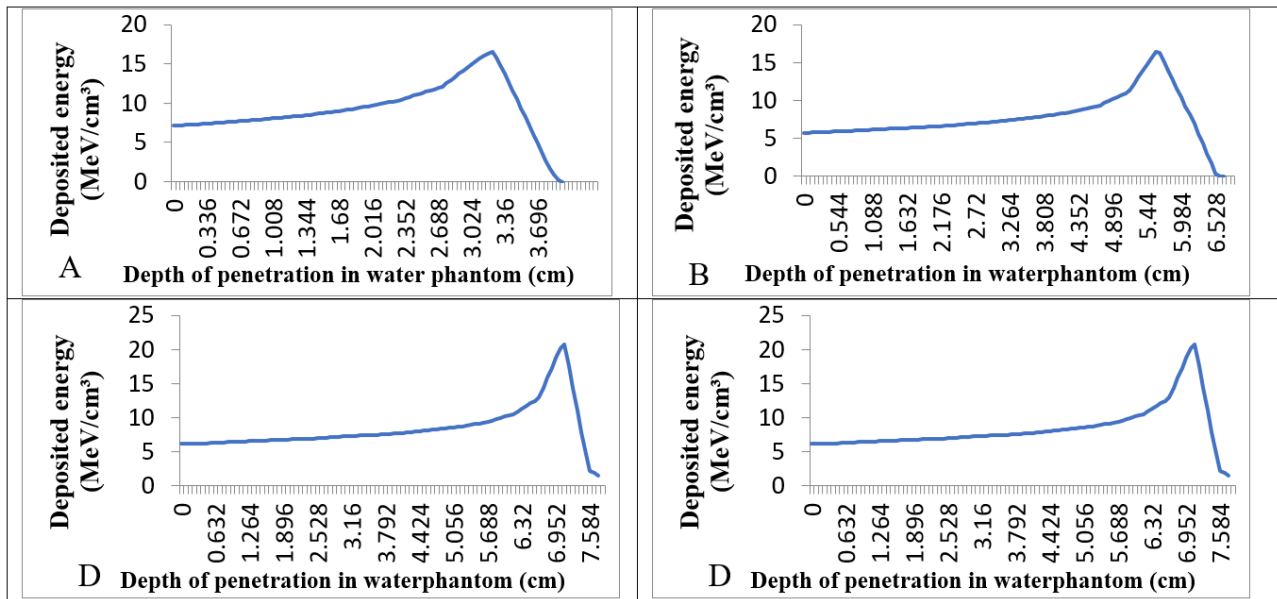


Figure 6: Bragg peak curves for different source energies and beam radius: (a-b) energy variation, (c-d) radius variation

was investigated under two distinct scenarios. In the first scenario, a 9-cm-thick homogeneous phantom consisting of bone and lung tissues was modeled, and the results for both media were compared. A monoenergetic proton beam with an energy of 50 MeV was used. The resulting two-dimensional penetration depth distributions were generated using Tecplot software. As shown in Fig. 5, due to the higher density and effective atomic number of bone tissue, proton penetration depth is reduced and the maximum dose occurs at a shallower depth compared to lung tissue (Verburg, 2015). In contrast, lung tissue, owing to its lower density, allows deeper proton penetration and results in a Bragg peak located at greater depths. In the second scenario, a heterogeneous layered phantom composed of bone, lung, and adipose tissues was constructed. The layer thicknesses were set to 0.5 cm for bone, 0.5 cm for lung, and 11 cm for adipose tissue. Simulations were performed using a 50 MeV proton beam, and the resulting two-dimensional penetration depth distribution was extracted and analyzed using Tecplot software.

3.2 Effects of Source Energy and Beam Radius on Proton Beam Behavior

Based on the simulation results, increasing proton source energy leads to a reduction in deposited energy and maximum absorbed dose, while significantly increasing beam penetration depth (Gottschalk, 2018). This behavior is illustrated in Figs. 6-A and 6-B, which present the Bragg curves for a fixed beam radius of 1 cm at proton energies of 70 MeV and 90 MeV. As shown, increasing energy results in a deeper shift of the Bragg peak along the penetration axis, accompanied by a decrease in the peak dose value. In contrast, variations in beam radius primarily affect the magnitude of the deposited energy without significantly altering the penetration depth. This effect is demonstrated in Figs 6-C and 6-D, where Bragg curves are shown for a constant proton energy of 100 MeV and beam radii of 0.7 cm and 0.9 cm. Increasing the beam radius reduces the height of the Bragg peak, while its position remains nearly unchanged. Overall, the results indicate that proton source energy is the dominant factor govern-

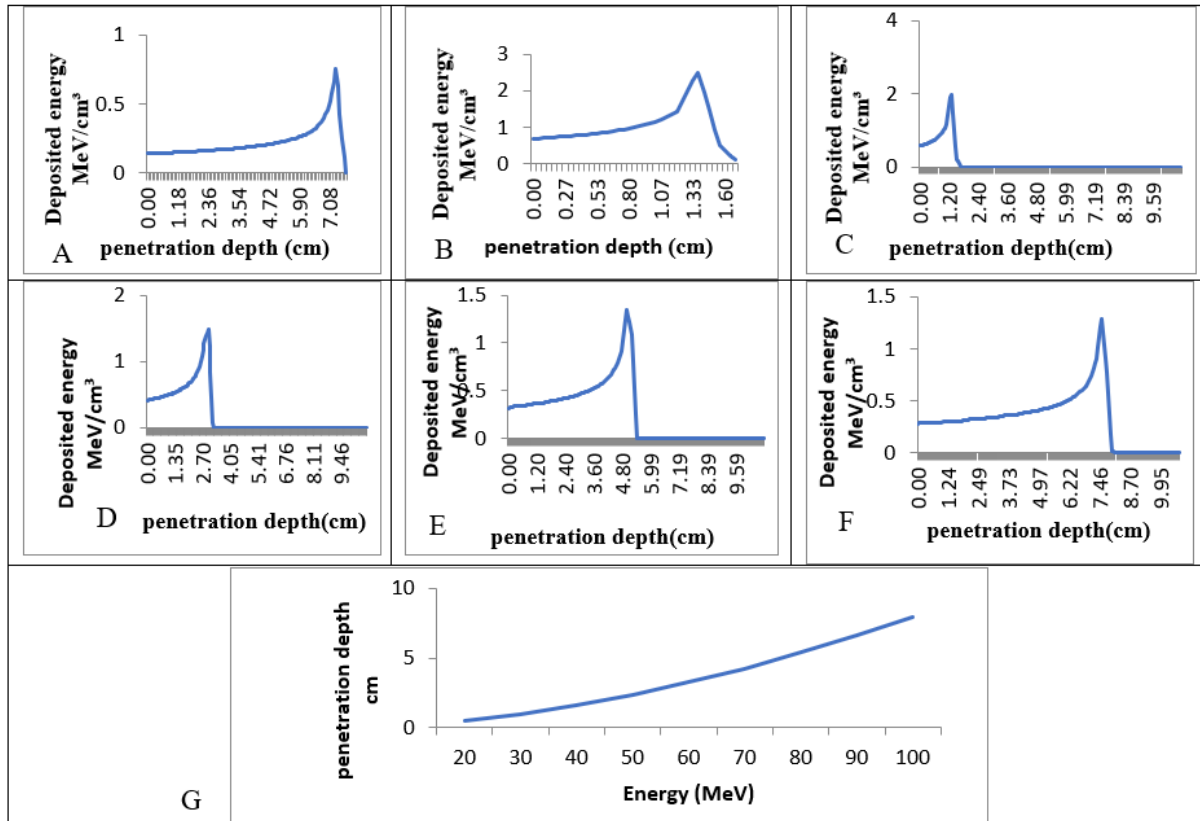


Figure 7: Bragg curves showing deposited energy as a function of penetration depth in lung and bone tissues. (A, B) Comparison of lung and bone tissues at 50 MeV; (C-F) bone tissue for proton energies of 40, 60, 80, and 100 MeV, respectively; (G) deposited energy profiles over the proton energy range of 20-100 MeV.

ing beam penetration depth, whereas beam radius mainly influences the magnitude of dose deposition and the maximum absorbed dose. These findings highlight the distinct roles of source energy and geometric beam parameters in shaping proton dose distribution within the medium.

3.3 Variations in Tissue Properties

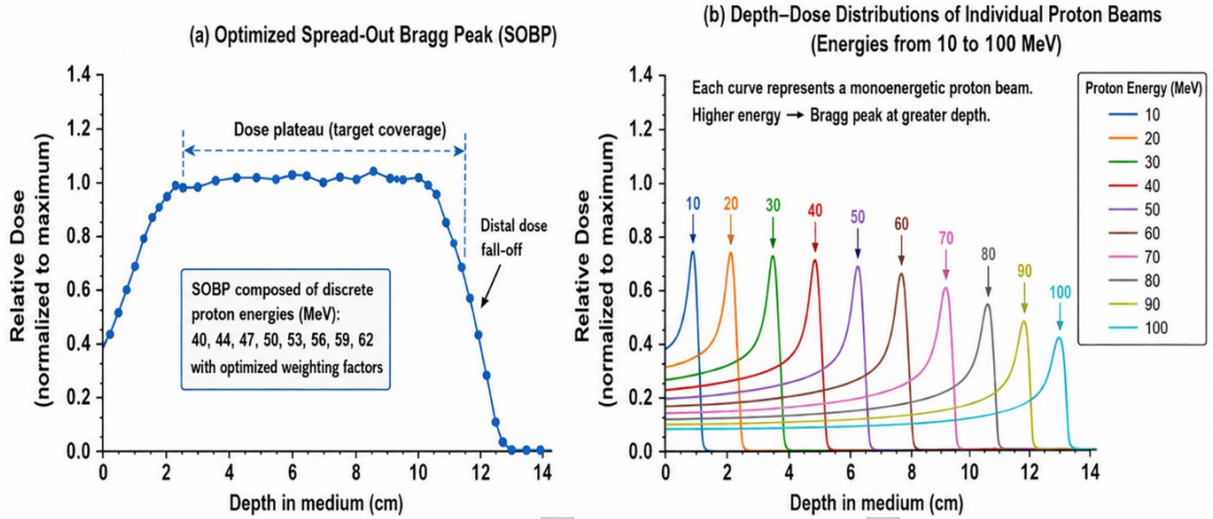
As tissue density increases, proton beam penetration depth decreases due to the greater number of interactions and enhanced energy loss within denser media. Consequently, higher-density tissues exhibit larger peak absorbed doses and increased energy deposition along the proton path (Schneider et al., 1996). This effect can be observed by comparing the Bragg curves obtained in lung and bone tissues (Figs. 7-A and 7-B). The initial proton energy also plays a crucial role in determining both the penetration depth and the characteristics of the Bragg peak. In bone tissue, proton energies of 40, 50, and 60 MeV produce Bragg peaks near the end of the proton range (Figs. 7-B to 7-D). Increasing the energy shifts the Bragg peak toward greater depths while reducing its amplitude as the deposited energy is distributed over a longer path length. The same trend is observed for proton energies of 80 and 100 MeV, where the Bragg peak occurs at even larger depths with a further decrease in peak height (Figs. 7-E and 7-F). A broader evaluation over the energy range of 20-100 MeV (Fig. 7-G) shows that the absorbed dose gradually increases with depth,

reaches a maximum near the end of the proton range, and then falls sharply beyond the Bragg peak. As proton energy increases, the Bragg peak shifts deeper into the medium, becomes broader, and exhibits a lower maximum value. These results demonstrate the combined influence of tissue density and proton energy on Bragg peak characteristics, highlighting that higher proton energies lead to deeper penetration and a more extended energy deposition profile within the tissue.

The results presented in Table 1 demonstrate that the presence of high-atomic-number impurities significantly affects proton transport characteristics within adipose tissue. The incorporation of gold, lead, and uranium increases the effective density and stopping power of the medium, leading to a progressive reduction in proton penetration depth relative to pure adipose tissue (Tabbakh, 2024). As shown, increasing proton energy leads to deeper penetration along the Z-axis and shifts the Bragg peak region toward greater depths, while the lateral dose profile remains largely unchanged. In addition, the profile slope ($\tan(\alpha)$) decreases in the presence of impurities, suggesting stronger lateral scattering and a broader spatial distribution of the proton beam. The magnitude of these effects becomes more pronounced with increasing atomic number, reflecting the greater interaction probability of protons in denser and higher-Z materials. Consequently, both the range and dose distribution of the proton beam are modified by the presence of impurities. These results

Table 1: Comparison of deposited energy, penetration depth, and profile slope of the proton beam in pure adipose tissue and adipose tissue containing gold, lead, and uranium impurities.

Description	Penetration depth (cm)	Deposited energy (MeV.cm ⁻³)	Slope of the profile (tan(α))
Three layers of adipose tissue	5.07	1.64	0.023
Three layers of adipose tissue with gold impurity	5.03	1.61	0.022
Three layers of adipose tissue with lead impurity	5.02	1.60	0.022
Three layers of adipose tissue with uranium impurity	5.01	1.59	0.021

**Figure 8:** (a) Optimized SOBP obtained by combining proton beams with discrete energies of 40, 44, 47, 50, 53, 56, 59, and 62 MeV. (b) Depth-dose distributions (Bragg curves) of individual proton beams with energies between 10 and 100 MeV, employed in the construction of a 12 cm-wide SOBP.

indicate that even low concentrations of high-Z materials can influence proton beam behavior and alter dose deposition patterns. Therefore, local compositional variations and material heterogeneities should be considered when evaluating proton range and dose distributions in proton therapy applications. Previous studies on proton beam interactions have primarily focused on macroscopic tissue heterogeneities such as bone, lung, and soft tissue, where density variations occur at the organ level (Vestergaard et al., 2023). In contrast, the present work introduces an additional level of complexity by considering micro-scale high-atomic-number (high-Z) impurities (gold, lead, and uranium) embedded within adipose tissue. Such localized compositional perturbations have rarely been investigated in earlier Monte Carlo-based proton therapy studies. Most existing literature assumes homogeneous tissue composition or standard ICRU-based material definitions, where elemental variations at the microscopic level are neglected. The results of this study demonstrate that even small fractions of high-Z inclusions can produce measurable changes in proton transport behavior, including increased stopping power, reduced penetration depth, and modifications in energy deposition and beam profile characteristics. This indicates that the Bragg peak is not only sensitive to large-scale anatomical heterogeneities but also to localized atomic-level variations in tissue composition. Therefore, the present study extends the conventional understanding of proton-matter interaction by quantifying the effect of embedded metallic impurities, which has not been explic-

itly addressed in previous simulation studies. To achieve a clinically useful dose distribution, a Spread-Out Bragg Peak (SOBP) was generated by superimposing multiple proton beams with discrete energies. The quality of the resulting SOBP depends not only on the selection of appropriate weighting factors (SP2), which determine the contribution of each energy component, but also on the accurate adjustment of the ERG and SI2 parameters controlling the energy spectrum and shape of the individual Bragg peaks. Proper optimization of these parameters enables the formation of a broader and more uniform dose plateau within the target region while maintaining the advantageous distal fall-off characteristic of proton therapy.

3.4 SOBP Formation

A fundamental requirement in proton therapy is the creation of a dose distribution capable of covering the entire tumor volume while preserving the characteristic distal dose fall-off of proton beams. Because a monoenergetic proton beam produces a narrow Bragg peak, it cannot provide a uniform dose across targets with finite thickness. To overcome this limitation, a Spread-Out Bragg Peak (SOBP) is generated through the superposition of multiple proton beams with different initial energies. The formation of an SOBP requires careful optimization of several beam parameters (Lomax, 2008). In addition to determining appropriate SP2 weighting factors, which define the relative contribution of each energy component

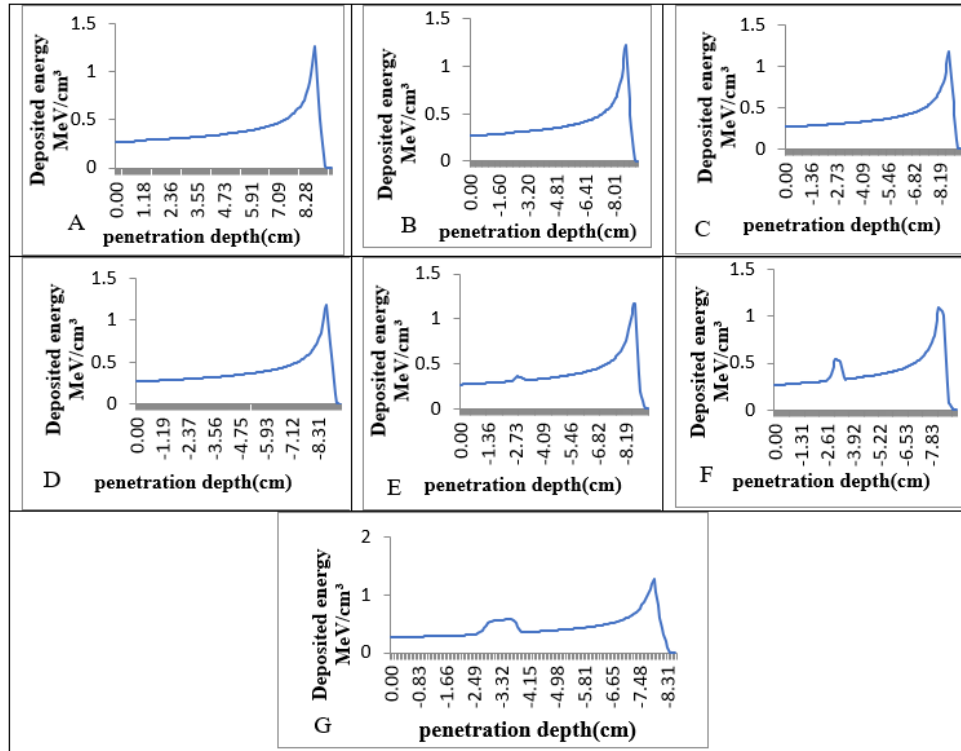


Figure 9: Depth-dose profiles of a 108.8 MeV proton beam in a 12 cm thick phantom for different heterogeneous configurations: (A) homogeneous water equivalent phantom (reference case); (B) and (D) high density bone layers; (C), (E), and (F) low density regions including air cavities or lung equivalent materials; and (G) multiple heterogeneous layers along the beam path. Material heterogeneity induces proximal or distal shifts of the Bragg peak and alters its height, width, and overall depthdose morphology.

to the composite dose distribution, accurate selection of ERG values (discrete proton energies) and SI2 parameters is necessary. These parameters govern the position and shape of the individual Bragg peaks and therefore directly influence the uniformity of the resulting SOBP. Proper adjustment of these quantities ensures adequate overlap among neighboring Bragg peaks and reduces dose inhomogeneities within the treatment region. Figure 8 illustrates the procedure used to construct the SOBP. Figure 8-b presents the depth-dose distributions obtained from individual proton beams with energies ranging from 10 to 100 MeV in a medium with a thickness of 12 cm. Each curve exhibits a characteristic Bragg peak whose position moves progressively deeper into the medium as the initial proton energy increases. Consequently, higher-energy protons deposit their maximum energy at greater depths, providing the basis for generating a broadened therapeutic dose region.

Using these individual depth-dose profiles, an optimized SOBP was produced by combining selected proton energies of 40, 44, 47, 50, 53, 56, 59, and 62 MeV with suitable weighting factors. The resulting composite distribution, shown in Fig. 8-a, exhibits a relatively flat dose plateau over the prescribed target depth. In contrast to the sharp and localized peaks associated with single-energy proton beams, the superimposed distribution delivers a nearly uniform absorbed dose throughout the treatment volume. The optimized SOBP provides improved target coverage while maintaining the inherent advantage of proton therapy, namely the rapid dose reduction beyond

the distal edge of the target. Such a dose distribution enables accurate irradiation of tumors with finite thickness and reduces unnecessary exposure of surrounding healthy tissues. Therefore, optimization of the energy spectrum and weighting factors plays a crucial role in achieving clinically acceptable dose uniformity and maximizing the therapeutic effectiveness of proton beam therapy.

3.5 Effects of Material Heterogeneity on the Bragg Peak

To evaluate the influence of material heterogeneity on proton beam behavior, simulations were conducted using a 12-cm-thick phantom irradiated by a 108.8 MeV proton beam. The resulting depthdose distributions for various heterogeneous configurations are presented in Figs. 9-A to 9-G. Figure 9-A corresponds to a homogeneous water-equivalent phantom and serves as the reference condition. Under this configuration, the Bragg peak is located at its expected depth, reflecting the nominal range of the incident proton beam. The introduction of dense materials, such as bone layers, along the beam trajectory (Figs. 9-B and 9-D) causes the Bragg peak to shift toward shallower depths. This behavior is attributed to the higher stopping power of dense media, which accelerates proton energy loss and consequently shortens the beam range. In contrast, configurations containing low-density regions, including air cavities and lung-equivalent materials (Figs. 9-C, 9-E, and 9-F), exhibit an increase in proton penetration depth. Because these materials provide less resis-

Table 2: Dependence of proton penetration depth and Bragg Peak position on the location and type of Heterogeneous tissues along the beam path.

Heterogeneous Tissue Position (based on penetration depth water phantom) - 8.69 cm Reference: Water Phantom	Depth Range (cm)		Thickness (cm)
	8.69-0.5= 8.19	8.69+0.5= 9.19	1
	8.69-0.25= 8.44	8.69+0.25= 8.94	0.5
	8.69-0.05= 8.64	8.69+0.05= 8.74	0.1

tance to proton transport, energy deposition occurs over a longer path length, resulting in a distal displacement of the Bragg peak relative to the homogeneous reference case. Beyond changes in peak position, material heterogeneity also affects the overall shape of the depthdose distribution. Variations in peak height, width, and gradient are observed across the investigated configurations, indicating that local differences in material composition can alter the spatial pattern of energy deposition. Such distortions may influence dose uniformity within the target volume and should therefore be considered during treatment planning. The most pronounced effect is observed in Fig. 9-G, where multiple heterogeneous layers are distributed along the proton path. In this case, the combined influence of materials with different densities produces a more complex depth-dose profile characterized by increased fluctuations and reduced uniformity. These findings demonstrate that heterogeneities can significantly modify both the location and morphology of the Bragg peak, emphasizing the importance of accurate tissue characterization in proton therapy dose calculations.

As shown in Table 2, the shift in the Bragg peak position is attributed to variations in the stopping power of heterogeneous materials relative to water-equivalent tissue. When the proton beam traverses higher-density regions such as bone, the increased electron density enhances energy loss, leading to a reduction in penetration depth and a proximal shift of the Bragg peak. In contrast, passage through lower-density materials, including air cavities or lung tissue, reduces the stopping power, allowing protons to retain their energy over longer distances and resulting in a deeper Bragg peak position. This dependence, commonly referred to as the heterogeneity effect, emphasizes the importance of accurately representing material composition along the beam path in proton therapy treatment planning. Neglecting these variations may compromise the accuracy of range prediction and ultimately lead to suboptimal dose delivery to the target volume or unintended irradiation of surrounding healthy tissues.

The presence of heterogeneous materials significantly influences key parameters of the Bragg curve, including the penumbra, full width at half maximum (FWHM), and peak position, in both the plateau and Bragg peak regions. These effects lead to a reduction in dose uniformity along the proton beam path, particularly when high-density materials are located near or within the Bragg peak region. In such cases, the peak is attenuated, its amplitude decreases, and the position of maximum dose is displaced. Failure to properly incorporate heterogeneity effects into treatment planning can result in a mismatch between the calculated and actual dose distributions, thereby compromising treatment accuracy. Moreover, the presence of het-

erogeneities within the plateau region may hinder the dose buildup toward the tumor, reducing target coverage while potentially increasing unintended irradiation of proximal or distal healthy tissues. Comparative analysis based on Monte Carlo simulations demonstrates a clear dependence of Bragg peak characteristics on the type and density of materials along the beam path. These findings emphasize the necessity of accurately determining and correcting the Bragg peak position relative to the tumor location in proton therapy to ensure optimal dose delivery.

4 Conclusions

Proton therapy enables highly localized radiation dose delivery; however, tissue heterogeneities and high-atomic-number (High-Z) impurities can modify proton transport and dose deposition. In this study, Monte Carlo simulations demonstrated that increasing proton energy increased the proton penetration depth and shifted the Bragg peak toward greater depths, whereas increasing the beam radius primarily reduced the Bragg peak amplitude without substantially changing its position. For example, increasing the proton energy from 70 to 90 MeV resulted in a deeper Bragg peak, while variation of the beam radius from 0.7 to 0.9 cm at 100 MeV mainly broadened the lateral dose distribution. The quantitative results further showed that the presence of High-Z impurities reduced the proton penetration depth from 5.07 cm in pure adipose tissue to 5.03, 5.02, and 5.01 cm for gold, lead, and uranium impurities, respectively. In parallel, the deposited energy decreased from 1.64 MeV/cm in pure adipose tissue to 1.61, 1.60, and 1.59 MeV/cm in the presence of gold, lead, and uranium, corresponding to reductions of approximately 1.83%, 2.44%, and 3.05%, respectively. The profile slope ($\tan(\alpha)$) also decreased from 0.023 for pure adipose tissue to 0.022, 0.022, and 0.021 for gold, lead, and uranium, respectively. These quantitative changes indicate that increasing the atomic number of the impurity was associated with progressively greater attenuation and modification of proton transport. Furthermore, simulations of heterogeneous tissue configurations showed that high-density materials such as bone shifted the Bragg peak toward shallower depths, whereas low-density materials such as lung and air shifted it toward greater depths. The optimized SOBP generated using proton energies of 40, 44, 47, 50, 53, 56, 59, and 62 MeV produced a relatively uniform dose distribution across the target region while preserving the distal dose fall-off. Overall, the numerical findings demonstrate that even localized High-Z inclusions and tissue heterogeneities can measurably alter proton range and energy deposition. Incorporating these effects into Monte Carlo-based dose calculations can there-

fore improve the accuracy of proton range estimation and dose delivery in heterogeneous clinical environments.

Conflict of Interest

The authors declare no potential conflict of interest regarding the publication of this work.

Funding

The authors declare that no funds, grants, or other financial support were received during the preparation of this manuscript.

References

- Baumann, K.-S., Gomà, C., Wulff, J., et al. (2023). Monte Carlo calculated ionization chamber correction factors in clinical proton beams—deriving uncertainties from published data. *Physica Medica*, 113:102655.
- Chao, T.-C., Tsai, Y.-C., Chen, S.-K., et al. (2017). An MC-NPX2. 7.0 study of Bragg peak degradation owing to density heterogeneity patterns for a CGMH therapeutic proton beam. *Radiation Physics and Chemistry*, 137:121–124.
- Cheung, J., Aubry, J.-F., Yom, S. S., et al. (2009). Dose recalculation and the dose-guided radiation therapy (DGRT) process using megavoltage cone-beam CT. *International Journal of Radiation Oncology* Biology* Physics*, 74(2):583–592.
- Cohilis, M., Souris, K., Buti, G., et al. (2023). A spot-specific range uncertainty framework for robust optimization of proton therapy treatments. *Medical Physics*, 50(10):6554–6568.
- Durante, M. and Loeffler, J. S. (2010). Charged particles in radiation oncology. *Nature reviews Clinical oncology*, 7(1):37–43.
- Ekinci, F. and Bölükdemir, M. (2019). *The investigation of Bragg curve parameters and lateral scattering of proton and carbon beam in different energy in the water phantom*. 5th International Conference on Theoretical and Experimental Studies in Nuclear Applications and Technology, Amasya, Turkey, 2 - 04 May 2019, pp.73.
- Gottschalk, B. (2018). Radiotherapy proton interactions in matter. *arXiv preprint arXiv:1804.00022*.
- Holmes, J., Feng, H., Zhang, L., et al. (2024). Fast Monte Carlo dose calculation in proton therapy. *Physics in Medicine & Biology*, 69(17):17TR01.
- Jabbari, K. (2011). Review of fast Monte Carlo codes for dose calculation in radiation therapy treatment planning. *Journal of Medical Signals & Sensors*, 1(1):73–86.
- Jia, Y., Zhao, L., Cheng, C.-W., et al. (2015). Dose perturbation effect of metallic spinal implants in proton beam therapy. *Journal of Applied Clinical Medical Physics*, 16(5):333–343.
- Lane, S. A., Slater, J. M., and Yang, G. Y. (2023). Image-guided proton therapy: A comprehensive review. *Cancers*, 15(9):2555.
- Lomax, A. (2008). Intensity modulated proton therapy and its sensitivity to treatment uncertainties 2: the potential effects of inter-fraction and inter-field motions. *Physics in Medicine & Biology*, 53(4):1043–1056.
- Newhauser, W. D. and Zhang, R. (2015). The physics of proton therapy. *Physics in Medicine & Biology*, 60(8):R155–R209.
- Paganetti, H. (2025). *Proton therapy physics*. CRC press.
- Pettersson, E., Thilander-Klang, A., and Bäck, A. (2024). Prediction of proton stopping power ratios using dual-energy CT basis material decomposition. *Medical Physics*, 51(2):881–897.
- Schneider, U., Pedroni, E., and Lomax, A. (1996). The calibration of CT Hounsfield units for radiotherapy treatment planning. *Physics in Medicine & Biology*, 41(1):111–124.
- Tabbakh, F. (2024). Significance of the proton energy loss mechanism to gold nanoparticles in proton therapy: a Geant4 simulation. *Scientific Reports*, 14(1):24978.
- Tabbakh, F. (2026). Resolving the contradiction between simulation and experimental results of using gold nanoparticles in proton therapy. *Scientific Reports*, 16(1):8012.
- Verbarg, J. M. (2015). Reducing range uncertainty in proton therapy.
- Vestergaard, C. D., Muren, L. P., Elstrøm, U. V., et al. (2023). Tissue-specific range uncertainty estimation in proton therapy. *Physics and Imaging in Radiation Oncology*, 26:100441.

©2027 by the journal.

RPE is licensed under a [Creative Commons Attribution-NonCommercial 4.0 International License](#) (CC BY-NC 4.0).



To cite this article:

B. Valizadeh, E. Saniei, A. Mosayebi, S. P. Shirmardi, H. Daneshvar, B. Sepehri. Monte Carlo simulation of the effects of high-Z elemental impurities on proton therapy dose distribution. *Radiation Physics and Engineering*, In Press.

DOI:

To link to this article: