Applied Radiation and Isotopes 173 (2021) 109709

Contents lists available at ScienceDirect

Applied Radiation and Isotopes

journal homepage: http://www.elsevier.com/locate/apradiso

Monte Carlo simulation to assess free space and end-weld thickness variation effects on dose rate for a new Ir-192 brachytherapy source

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ARTICLE INFO

Keywords:
Iridium-192 seeds
Brachytherapy
Dosimetry
Monte Carlo simulations
Source production

ABSTRACT

A new Iridium-192 seed for brachytherapy is under development. Specific dose rate contribution by two different factors were evaluated: the effect from movement of the core in the free space within the seed and the effect of the end-weld thickness variation. Both were investigated through use of the Monte Carlo radiation transport code MCNP6 and an in-house routine programmed with MATLAB. Differences greater than 15% compared to results from the nominal seed were found near the source, indicating a significant dose variation.

1. Introduction

One of the most important aspects of radiation therapy is accuracy, meaning that the calculated dose is actually the one that is being delivered to the patient. Subjects like dosimetry checks with phantoms or *in-vivo* are largely discussed, but source fabrication errors and defects aren't approached frequently. These manufacturing issues are, most of the time, not easily (or not possible to be) resolved, and sources are produced and used without this evaluation. Those errors can result is dosimetry deviations that might be significant to the final radiation dose output.

In our research group, Rostelato developed a low-dose rate Iridium-192 wire to be used in cancer treatment (Rostelato, 1997). Mattos took the wire developed by Rostelato and encapsulated following the Iodine-125 silver wire model (Mattos, 2013). The group is now developing a semi-industrial laboratory located at Nuclear and Energy Research Institute (Brazil) to fabricate the new seed model that consists in a biocompatible titanium shell laser-welded in both ends containing the Iridium-192 wire core. Titanium is used as encapsulation since it is already implemented for Iodine-125 seeds at this facility and the main objective with the development of this new model is to achieve a low cost of production (so that the national seeds can be an economically viable alternative to imported models and be adopted by local hospitals through the public national health care system, SUS).

Iridium-192 is being used for brachytherapy since ca. 1960 (RJ and M, 1990), with publications from 1966 by Henschke et al. (1966) suggesting its use due to the high specific activity that can be achieved in source production. There is at least one dosimetric routine published about this radionuclide from the same year (Hall et al., 1966). The original TG-43 protocol lists Iridium-192, as well as Iodine-125, as the radionuclides most used in the United States for interstitial brachytherapy (Ravinder et al., 1995). Towards the end of the twentieth century, Monte Carlo simulations became a common practice to account for dosimetric parameters of brachytherapy seeds, Iridium-192 included (Ballester et al., 1997; Pérez-Calatayud et al., 1999; Wang and Sloboda, 1998), and is recommended by the active upgrade of protocol TG-43 (Rivard et al., 2004).

Iridium-192 decays to Platinum-192 via beta emission (95.24%) and to Osmium-192 by electron capture (4.76%), with a half-life of 73.83 days (National Nuclear Data Center. Brookhaven National Laboratory, 2020). Only gamma and x-ray emission are expected to contribute to treatment, as the titanium shell shields the beta particles emitted. Iridium-192 is produced by neutron activation of Iridium-191, which is stable and of natural occurrence. For our source, the activation is done in the research reactor IEA-R1 of the Nuclear and Energy Research Institute (Brazil).

Brachytherapy dose calculations rely on previous measurements of the dose rate around the source. These are usually done before the seed

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https://doi.org/10.1016/j.apradiso.2021.109709
Received 26 July 2020; Received in revised form 20 December 2020; Accepted 26 March 2021
Available online 8 April 2021
0969-8043/

becomes commercially available, following a dosimetry protocol. The majority of protocols take into account inhomogeneities on patient's tissue, source self-attenuation and the finite dimensions of patient (Beaulieu et al., 2012). The most commonly used is still the Task Group 43 Report (TG-43) from AAPM (American Association of Physicists in Medicine), published in 1995 and updated in 2004, also known as TG-43 U1 (Ravinder et al., 1995; Rivard et al., 2004). TG-43 U1 is widely used due to easy implementation in clinical practice. It relies on a water-based dosimetry using a 30 cm phantom of water-equivalent material that considers enough backscattering material so that the patient and its surroundings are treated as an infinite homogeneous water medium.

One topic usually not considered is the variation on the internal dimensions of seeds due to the inaccuracy in its production. Ideally, all sources should be equal to the one used during dosimetric characterization to match SK (air-kerma strength) value. Otherwise, they should be measured for different seed production batches to guarantee validity of previous dosimetry calculations. Monte Carlo simulations have been used to quantify the uncertainty of the dose distribution around an Iodine-125 seed due to construction limitations (Pantelis et al., 2013).

This present work aims to estimate if the welding and the free air space between the Iridium-192 wire and encapsulation do affect the final dose rate relevantly. If so, this work will contribute for the optimization of manufacturing procedures used in this new seed model. Results are presented in the format of mean values for dose rate at given points and their respective deviations.

2. Methodology

This work used simulations with MCNP6 code, developed by Los Alamos National Laboratory. Additional programming was executed with MATLAB®, such as input writing and output data reading. MATLAB® in-house routines were programmed for such tasks. Details on the simulation data are shown in Table 1 as well as spread on the text, in accordance to AAPM's TG-268 report, which is the reference to publication data for Monte Carlo simulations (Rogers et al., 2018).

Table 1
Monte Carlo simulation data following TG-268 publication protocol (Rogers et al., 2018).

Item	Description and References
Software	MCNP6 (1.0) (Pelowitz, 2013).
Hardware	A 7th gen Intel® dual core i5-7200U processor with 8 GB RAM (clock speed of 2.5 GHz, up to 3.1 GHz with Turbo Boost), leading to a total simulation time of circa 70 h (circa 30 min for each individual simulation).
Geometry	Source within a water sphere with radius of 15 cm, based on TG-43 U1 protocol (Rivard et al., 2004).
Materials	See Table 2 for materials and reference.
Source	As described and discussed in text and Fig. 2, based on the original design by manufacturer (Cardoso et al., 2017; Feher, 2014).
Physics and Transport	• Cross section data obtained from MCPLIB04, (known in-code as 04p or 84p for the updated version) (White, 2003); • Iridium-192 photon emission spectrum was obtained from Nuclear Data Sheets retrieved from the National Nuclear Data Center of Brookhaven National Laboratory (Baglin, 2012; National Nuclear Data Center. Brookhaven National Laboratory, 2020); • Default particle weight and energy cutoffs from MCNP6 were used, as well as default transport for secondary particles (secondary electrons were transported).
Scoring	• Tally FMESH4 was used with DE/DF card, providing average flux of particles over a cell, combined with mass-energy absorption coefficient data for water, allowing to estimate average energy deposited in medium (kerma), taken as numerically equal to absorbed dose since electronic equilibrium was considered; • Cylindrical geometry was used for FMESH tally; • Data presented in figures underwent a linear interpolation after transformation of coordinates to cartesian system; • A total of 10^8 particle-stories were executed, leading to a MCNP6-calculated type-A uncertainty below 1% for any given point. Impact of uncertainty is subject of this study and is debated along the text.
Analysis	Scored quantities were not filtered or de-noised. Since data was analyzed only as relative difference to reference case or as curve doses normalized by maximum dose (excluding pixels that coincide with the seed source), no further conversion was needed.
Validation	This work uses MCNP6, a well stablished radiation transport code, to discuss theoretical impact of variations on the source production that otherwise would be difficult to detect in experiment due to their specificities, so no validation against experimental data or other available codes was executed.

2.1. Simulation input data

The seed was modeled after its nominal dimensions (Mattos et al., 2010; Rostelato, 1997; Rostelato et al., 2014). However, there is no information regarding the end-weld dimensions, except it has the same sectional radius of the capsule outer wall. Since the welding system used was developed specifically for use by the Radiotherapy Sources Production Laboratory at Nuclear and Energy Research Institute (Brazil), more details of it were found either under literature (Feher, 2014; Feher et al., 2011) or by direct measurement of the seeds. A microscopy image of the welded tips is shown in Fig. 1. Some important topics regarding details on its geometry were noticed:

- The welding process yields different results depending on the side being welded. Usually, when the empty titanium tube receives the first weld, an almost perfect spheroid is formed with half its mass extending beyond the hollow section. Then the Iridium-192 wire is accommodated inside the titanium tube, before the second end is welded. Due to the pressure inside the tube, the second end-weld results in a different shape, with the outer part identical to the hemispheroid of the other tip, but the internal part being deformed into a slightly concave or plane shape. The plane shape was considered for this model, as shown in Fig. 2;
- Amongst the seeds selected for this test by criteria like roundness, symmetry, and weld damage, a considerable variation on the dimensions was found (Feher, 2014), thus reinforcing the need of a dosimetric analysis. The nominal length of the seed, 4.5 mm, has hemispheroidal tips with semidiameter of 0.25 mm on its longitudinal axis, but the variation on the welding may lead to lengths of up to 4.67 mm (measured of a batch of 70 samples). Since there is no significant deviation on the length of the original outer capsule, this increase was attributed solely as variation of the weld.

Originally, the manufacturer proposed a symmetrical geometry, but due to the different end-weld thicknesses achieved, visible in Fig. 1, a more realistic approach was considered when modeling the source.

For simulation, the surrounding medium was considered as a 15 cm radius water sphere to assure ideal backscattering conditions, following TG-43 U1 recommendations. The final model used, as well as the material composition, are shown in Fig. 2 and Table 2, respectively.

Since the titanium encapsulation shields all beta radiation emitted from the core, only transport of photons and secondary electrons generated by photon interactions were considered. Dose per photon was calculated using tally *FMESH4 combined with DE/DF card containing the mass-energy absorption coefficient data for water, allowing to score average energy deposited in medium (collisional kerma), and considering electronic equilibrium to assume its value to be numerically equal to dose. Results were analyzed point-by-point following the TG-43 U1 coordinate system, with θ angles varying from 0° to 180°, 10° step, and r distances up to 5 cm, with a 0.1 cm step.

Iridium-192 emission spectrum was taken from literature (Baglin, 2012). A total number of 10^8 particle-stories were simulated for each

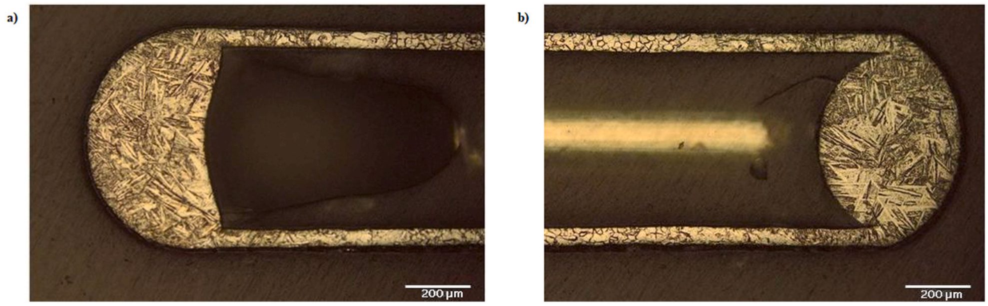

Fig. 1. Tip of the titanium tube laser welded; a) second-welded tip, collapsed; b) first-welded tip, ellipsoidal. Reproduced from (Feher, 2014) (no permission needed).

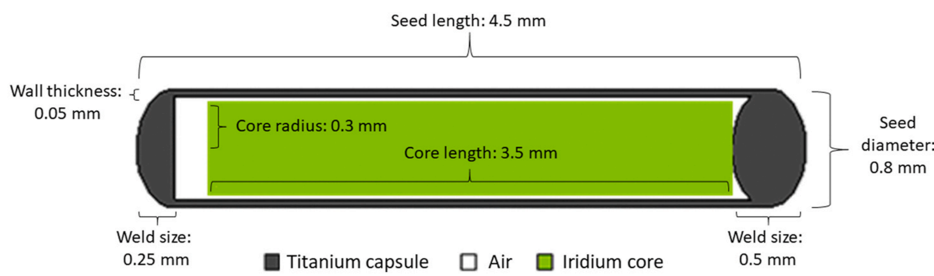

Fig. 2. Iridium-192 seed model used.

Table 2
Materials composition used for Monte Carlo simulation.

Material	In model	Composition	Density
Iridium	Seed core	100% Ir	22.56 g/cm^3
Air [a]	Seed free-space	0.0124% C 75.5268% N 23.1781% O 1.2827% Ar	1.20479 × 10^{-3} g/cm^3
Titanium	Seed encapsulation	100% Ti	4.54 g/cm^3
Water	Surrounding medium (15 cm water sphere)	100% H_2O	1 g/cm^3

[a] Dry air (near sea level) composition, taken from NIST STAR database (National Institute of Standards and Technology, 2019).

run, leading to a MCNP calculated type An uncertainty on dose no higher than 1% for any point.

2.2. *Variation of parameters and statistical analysis*

The statistical approach used in this work was based on Pantelis et al. (2013). The effect of the variation on two parameters (free space and end-weld thickness) was analyzed in this work. For each one, 70 different simulations were performed, and the final result for dose at each point was calculated as the average of all 70 values at that point. Results are presented separately for each parameter. If the mean deviation values found for any parameter are significant, they should be considered relevant to the final dose by propagation of uncertainty.

The data for end-weld thickness variation was taken from the welding process developer (Feher, 2014). A batch of 70 seeds was physically measured (no need for randomly generated new values). The nominal value of L = 4.5 mm for seed length was found to be not the actual mean value, but rather the minimum length. The maximum length measured in this batch was L = 4.67 mm, the mean value was L = 4.57 ± 0.04 mm, and mode L = 4.55 mm. To account for length increase on both ends, a parcel of 4.00 mm was subtracted from each value of L, and the result was divided by two, considering both end-welds to have always the same thickness (as an approximation). Two images of seeds modeled with different welds are shown in Fig. 3. To keep the core position geometrical center coincident with the seed geometrical center, thus not variating the core position in this parameter analysis, it was considered that the increase on the end-weld thickness could make it trap the core, as noted in Fig. 3a, even though the core is actually placed within the shell after the first welding, thus being displaced towards the second end-weld in these cases.

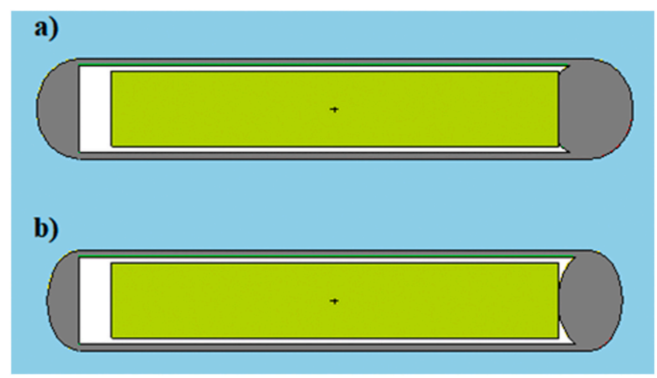

Fig. 3. Two seeds modeled with different end-weld thickness. a) 4.67 mm length seed, the weld traps the wire end; b) 4.50 mm length seed, weld occupies the free space, not trapping the wire.

For the variation of the core position, there was no previous dataset. However, considering that the seed may achieve different orientations during clinical practice, and unless the core ends up welded to the outer tube by chance, it is reasonable to assume the core can be anywhere on the free air space within the seed. Considering this, a MATLAB® in-house routine was programmed to write 70 different inputs of MCNP varying the core position to any possible free space on the seed, except it always keeps the same orientation.

The results were analyzed also with MATLAB®. The two main aspects to be discussed are mean value for each point, which can represent a deviation from reference value, obtained with the nominal seed; and standard deviation from the sample, which indicates the expected variation of the dose with the disparity of that parameter.

3. Results and discussion

Dose rate values for the nominal seed model are shown in Fig. 4. Results averaged by each sample of 70 seeds, with varying weld thickness and core position, are compared to the reference case. Data comparison between reference case and variation of the core position is presented using the anisotropy function in Fig. 5. Since results for varying weld thickness are visually indistinguishable from results from the reference case, they were omitted from Fig. 5. Type-A uncertainty on the averaging for each parameter is discussed later, as it is relevant to the scope of this work. The deviation from nominal seed value is shown in Fig. 6, with overall uncertainty no greater than 1.42% for any shown point.

As seen in Fig. 6a, variation on weld thickness within the observed range does not impact significantly the dose rate profile, with relative difference from the nominal seed majorly within ±0.5%. The pattern observed can be inferred to result from the fact that the weld thickness for the nominal seed is actually the shortest measured in practice. As the weld thickness increases, dose in the longitudinal axis of the seed decreases due to attenuation. As the right-side of Fig. 6a represents the ellipsoidal welding, it has double the amount of titanium than the left-side, leading to an even greater attenuation for that tip of the source. Additionally, there is a slightly tilt to higher doses for θ around 90°, probably due to more photons of the source scattered to this direction.

Different positions assumed by the core impacts dose rate profile more than different weld thicknesses, as can be seen in Fig. 5, where the anisotropy function for the mean value of the core-displaced simulation results is more deviant from nominal model near angles of 0° and 180°, being more discrepant in small distances. This behavior can also be seen in Fig. 6b, where relative difference to the reference case is of an order of magnitude ten times higher than the data shown in Fig. 6a, for the end-weld thickness variation. A significant shift of the dose rate along the longitudinal axis is observable, with an increase on the dose on the second-welded tip and a decrease on the first-welded tip, to the right. The nominal seed was originally supposed to be symmetrical, but since this is not the case observed in microscopy, the collapsing of the weld in the left tip leaves more empty room for the core to be displaced to that direction, leading to differences of up to 18% around the tip of the seed, and around ±2% for the majority of the analyzed points with $r < 1$ cm, except around $\theta = 90°$, which is largely unaffected by displacement of the core.

The overall agreement seen in Fig. 6a indicates that influence on final dose rate due to differences on the end-weld thickness is very low and statistically negligible. Those are important information for the seed manufacturer. It also shows that, within the range of length L sampled, nominal value of $L = 4.5$ mm can be used for dosimetric calculations even if it not corresponds to the actual mean value without incurring on relevant impact on the calculated dose. On other hand, the effect on dose by different positions of the core is not negligible. The high relative difference in the sample shows there is a relevant impact on dose, which decreases with distance as expected by geometrical reasons. Depending on position of the core, the relative difference between two simulations is as higher as 18% at point p = (3 mm, 180°). The relative differences increase with angular variation, peaking at 0° and 180°, also for geometrical reasons, as deducible from the definition for the geometry function from TG-43 U1 (Rivard et al., 2004). With the core movement on the longitudinal axis, the distance between a point of interest at these angles and the tip of the core is significantly reduced or increased, resulting on a significant impact. This result shows that dosimetry calculations considering a stationary core is not totally reliable.

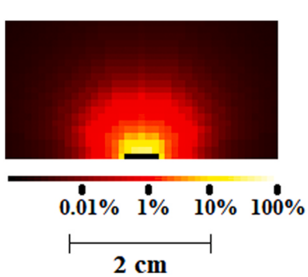

Fig. 4. Dose rate profile for a nominal seed.

Another aspect that should be taken into account is the deviation between dose rates obtained from different seeds within the same batch, calculated as the standard deviation from the averaging of dose rates at each point, which is shown at Fig. 7. If the deviation is negligible, one may simply change the nominal value for a given parameter to reach a better agreement with the reference dose rate profile. However, if the deviation is significant, its impact on the dose rate profile should be considered by propagation of uncertainty, following TG-43 U1 recommendations (section IV.C) that strongly encourages researchers to account rigorously for different sources of uncertainty.

Again, the welding variation results in a case of less concern, as the majority of the points at close distance lies within a standard deviation of ±0.1%. Nonetheless, variation on the core position cannot be well represented even changing nominal seed description, since different dose rate profiles obtained varying this parameter do not agree well, with standard deviations of up to 10% around the source. It is also important to take in consideration that core displacement is not a parameter under direct control of manufacturers, implying more concern to its practical use, unless the source manufacturer can improve the immobility of the wire inside the source by fastening it.

4. Conclusions

This work aimed to analyze parameters relevant to dosimetry of a new brachytherapy seed model not taken into account on TG-43 U1 protocol, although the TG-43 U1 coordinate system was used, as well as its formalism of dose to water. One objective pursued was to prevent future inconsistencies when this protocol will be applied for both experimental and Monte Carlo dosimetry, assessing the effects of two parameters not usually observed.

The end-weld thickness was considered as a possible source of error to the final dose, but within the range of observed seeds in one batch produced, this variation does not lead to any statistically significant change to final dose. Core position inside the seed, on other hand, proved to be a relevant parameter to be taken into account for two aspects:

1) because the mean value for dose rates obtained from a set of 70 seeds modeled with core positioned randomly did not agree to the dose rate calculated from reference case, a shift on results was observed due to a higher probability of the core being displaced towards the second-welded end of the seed. This proved it is necessary to either develop a new way of keeping the core wire fastened within the tube or to remodel the nominal seed used for Monte Carlo dosimetry. Otherwise systematic errors may arise when comparing Monte Carlo simulations with experimental data;

2) even within the set of randomly displaced cores, a great deviation from dose rate mean value was observed, especially close to the ends of the seed. Even if the core is correctly represented in Monte Carlo dosimetry, this displacement cannot be avoided neither in experimental dosimetry nor on clinical practice. They must be taken into account when calculating the propagation of uncertainty on dose rate profile around the seed, by mapping the deviation for each point of interest using Monte Carlo and them adding this deviation as another source of uncertainty. Tracking these effects before the full dosimetry is undertaken is highly desirable, preventing unexpected inconsistencies that would be hard to correct following strictly the TG-43 U1 protocol.

Although the results presented in this work are specific to this new seed model under development, the discussions may be of use by other manufacturers and researchers, since most seed models lack a guarantee

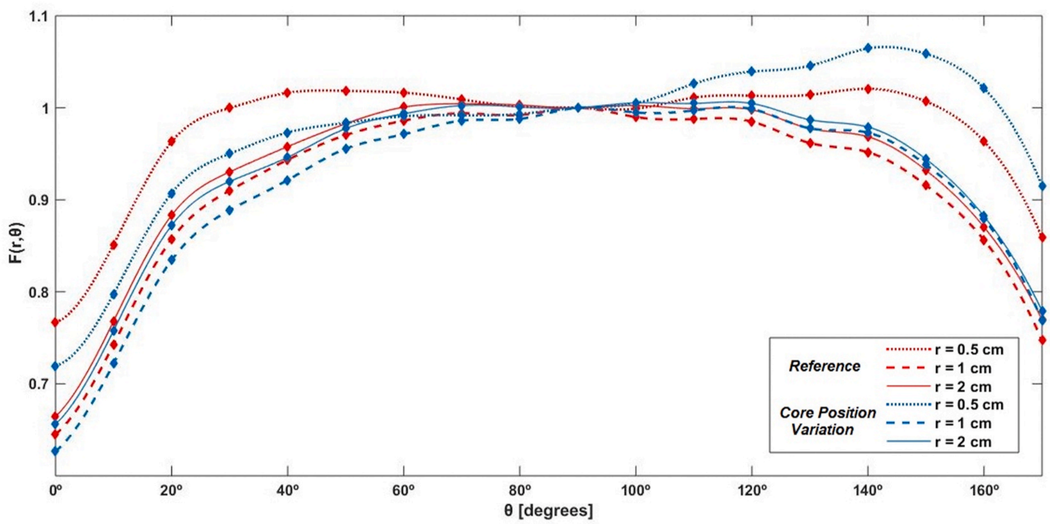

Fig. 5. Anisotropy function F(r,θ) for the reference case and for the mean value of the batch with varied core position, at radii 0.5, 1 and 2 cm.

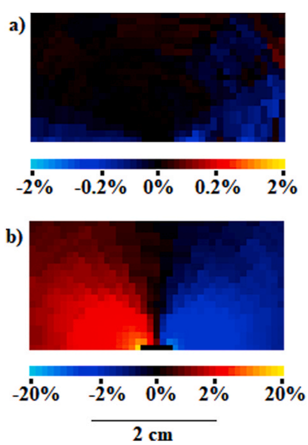

Fig. 6. Relative difference from nominal dose rate profile of the average dose for a) a batch of 70 seeds with varying weld thickness; b) a batch of 70 seeds with varying core position.

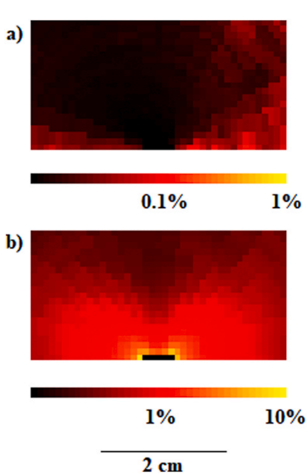

Fig. 7. Standard deviation for averaging dose rate for a) a batch of 70 seeds with varying weld thickness; b) a batch of 70 seeds with varying core position.

of the core position, which may be a relevant source of uncertainty usually not taken into account (both for calculated dose and agreement with experimental data).

Further work on this subject shall consider other parameters, like outer tube thickness and composition of materials. Also, reconsider the nominal seed model and, ultimately, realize the full TG-43 U1 protocol dosimetry considering all the effects previously observed.

Author statement

Lucas Verdi Angelocci: main work executor, writing, and simulation. Carla Daruich de Souza: corresponding author, writing, and simulation correction. Evaggelos Pantelis: writing, simulation main advisor. Beatriz Ribeiro Nogueira: simulation advisor. Carlos Alberto Zeituni: simulation advisor. Maria Elisa Chueri Martins Rostelato: work general advisor (Lucas PhD advisor).

Declaration of competing interest

All authors declare that are no financial and personal relationships with other people or organizations that could inappropriately influence their work.

Acknowledgments

This work was supported by:

- CAPES- Coordenação de Aperfeiçoamento de Pessoal de Nível Superior, BRAZIL [grant number 88882.333477/2019-01]
- IAEA- International Atomic Energy Agency [grant numbers BRA17013 and BRA6026]
- FAPESP- Fundação de Amparo à Pesquisa do Estado de São Paulo, BRAZIL [grant number 2018/18526-2]

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