Monte Carlo water-equivalence study of two PRESAGE® formulations for proton beam dosimetry

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Abstract. PRESAGE® is a radiochromic solid dosimeter which shows promising potential for 3D proton beam dosimetry. Since an idea dosimeter should be water-equivalent, total depth dose distributions in two PRESAGE® formulations irradiated by a 62 MeV proton beam were compared with that in water using GEANT4 Monte Carlo simulations. The dose delivered by secondary particles was also calculated. Our results show that after water-equivalent depth scaling, PRESAGE® can be considered water equivalent for dosimetry of a 62 MeV clinical proton beam.

1. Introduction

Polymer gel dosimeters are manufactured from radiation sensitive chemicals, which upon irradiation polymerize as a function of the absorbed radiation dose [1]. These gel dosimeters which record the radiation dose distribution in three-dimensions (3D) have specific advantages when compared to one-dimensional dosimeters and two-dimensional dosimeters [2]. These 3D dosimeters are radiologically soft-tissue equivalent [3] with properties that may be modified depending on the application. The 3D radiation dose distribution in polymer gel dosimeters may be imaged using magnetic resonance imaging (MRI) [4, 5], optical-computerized tomography (optical-CT) [6, 7], x-ray CT [8, 9], ultrasound [10, 11, 12] or vibrational spectroscopy [13, 14].

PRESAGE® is a radiochromic polyurethane based dosimeter containing leuco dyes and free radical initiators. Ionizing radiation darkens PRESAGE® and changes its optical density; hence, a quantitative evaluation of the optical absorbance change of PRESAGE® can provide a measure of 3D absorbed dose [15-18]. PRESAGE® has presented potential for dosimetry of proton therapy [18-22]. Proton therapy is an external radiation treatment which delivers vey localized high dose at the distal end of the beam (Bragg peak). Precise 3D dosimetry of proton beams is important to ensure of treating tumor with minimizing damage to the healthy surrounding tissues.

To be used for clinical dosimetry, ideally a dosimeter should be water equivalent. To be considered water equivalent for proton dosimetry, it should have a similar electronic mass stopping power and secondary particle production to water [23, 24].

The water equivalence of different PRESAGE® formulations has previously been investigated for x-ray radiotherapy [25-27]. In this study, total depth dose and dose delivered by secondary particles in

two different formulations of PRESAGE® by a 62 MeV proton beam are compared with those of water using Monte Carlo modeling.

2. Materials and Methods

Table 1 shows the chemical formula and fractional weight of two PRESAGE® formulations, one with the lower halogen content (formulation A), and water. To investigate water equivalency of PRESAGE® formulations, a model was developed based on the hadrontherapy advanced example in GEANT4 toolkit (a Monte Carlo code) [28] to calculate depth-dose profiles of a validated 62 MeV proton beam in two PRESAGE® formulations and water. Dosimeters and water were modeled as large cubic volumes ($10\times10\times10$ cm^3). Delivered dose was calculated along the central axis and laterally in a $4\times4\times4$ cm^3 cube which was divided into voxels of $0.2\times2\times2$ mm^3. The dose delivered by primary and secondary protons, secondary electrons and secondary neutrons was also calculated by setting the appropriate tracking ID number in the GEANT4 code. 2D cross-sectional total dose distributions were also calculated.

Water equivalent depth was calculated using the following formula based on IAEA report 398 and ICRU report 49 recommendations [24, 29]: Water equivalent depth = $z_m \cdot c_m$, where z_m is the material areal density (density-thickness) and c_m is a depth scaling factor defined as the ratio of the continuous slowing down approximation (CSDA) range of protons in water to the CSDA range of protons in a given material. CSDA ranges were estimated using our Monte Carlo simulated results.

Table 1: Chemical formula and fractional weight (w_k) for materials of interest.

Material	Formula	w_H	w_C	w_N	w_O	w_S	w_{Cl}	w_{Br}
PRESAGE® formulation A	$C_{1758}H_{3000}N_{121}O_{442}S_4Cl_{30}Br_1$	0.08850	0.6178	0.04960	0.2069	0.003800	0.03112	0.002300
PRESAGE® formulation B	$C_{481}H_{842}N_{30}O_{129}Cl_9Br$	0.08920	0.6074	0.04460	0.2172	-	0.03340	0.008400
Water	H_2O	0.1119	-	-	0.8881		-	-

3. Results

Figure 1 shows the calculated percentage dose versus depth for two PRESAGE® formulations and water. Protons deliver their dose more rapidly in the PRESAGE® formulations than in water and this can be attributed to the different chemical compositions which lead to the differences in stopping power. Dose delivered in PRESAGE® formulations A and B and water reaches its Bragg peak at 27.3 mm, 25.5 mm and 29.1 mm, respectively. Practical range (where dose reaches to the 10% of the Bragg Peak) of the 62 MeV proton beam is at 26.8 mm, 28.6 mm and 30.5 mm depth from the surface for PRESAGE® formulation A and B and water, respectively. As a result of these discrepancies, a water equivalent depth calculation is required to compare the depth dose of PRESAGE® formulations with water.
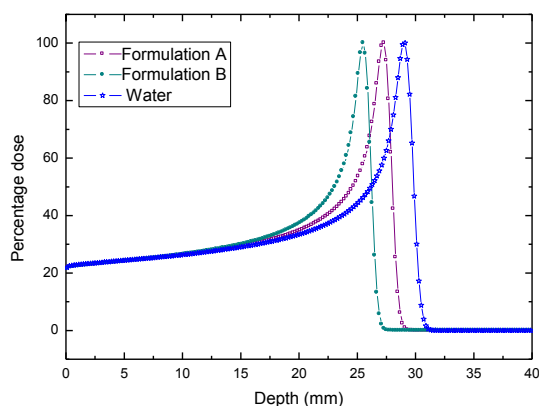
Figure1: Monte Carlo calculated total percentage dose versus depth for the two PRESAGE® formulations and water by a 62 MeV proton beam

The percentage contributions of dose delivered by secondary protons and electrons to the total dose are presented in figure 2. As expected, more than 95% of the total dose is delivered by the primary particles. Secondary protons and secondary electrons deliver less dose in PRESAGE® formulations compare to water over the entire range of the beam. Contributions of secondary protons and electrons in the total dose for formulation B is significantly lower than formulation A and water. Dose delivered by secondary neutrons is negligible in all the materials of interest for the 62 MeV proton beam.
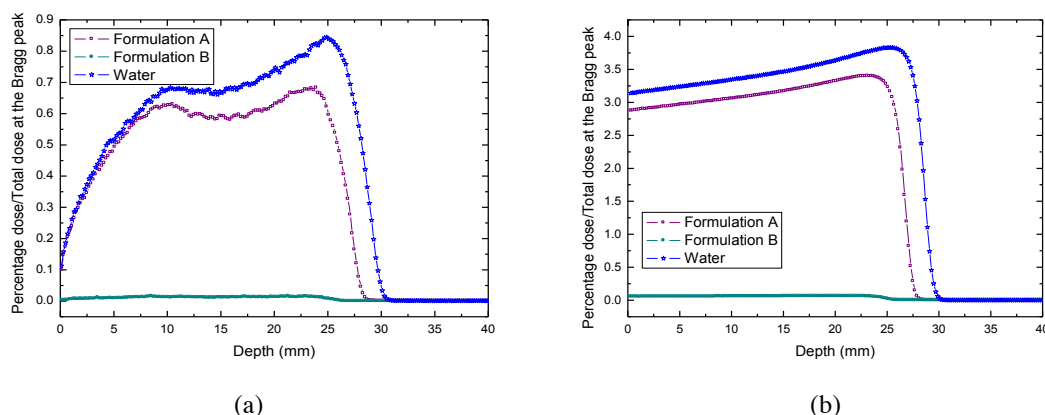

(a)   (b)

Figure 2: Monte Carlo calculated percentage dose normalized to the total dose at the Bragg peak versus depth for (a) secondary protons and (b) secondary electrons for two PRESAGE® formulations and water.

Figure 3 shows the Monte Carlo calculated percentage total dose for PRESAGE® formulations and water for a 62 MeV proton beam versus water equivalent depth. Also shown is the cross-sectional total dose distributions calculated at 29.5 mm water equivalent depth normalized to dose at the Bragg peak. Before the Bragg peak, dose delivered in PRESAGE® formulations is less than water by $\approx 2\%$ due to having less dose delivered by secondary particles. This trend is consistent with the calculated 2D cross sectional dose result. After the Bragg peak, less than 2% discrepancies from water is observable which can be attributed to the differences in the dose delivered by primary protons.

4. Conclusion
These results indicate that both PRESAGE® formulations investigated can be considered water equivalent for dosimetry of a 62 MeV proton beam if a water equivalent scaling is applied.
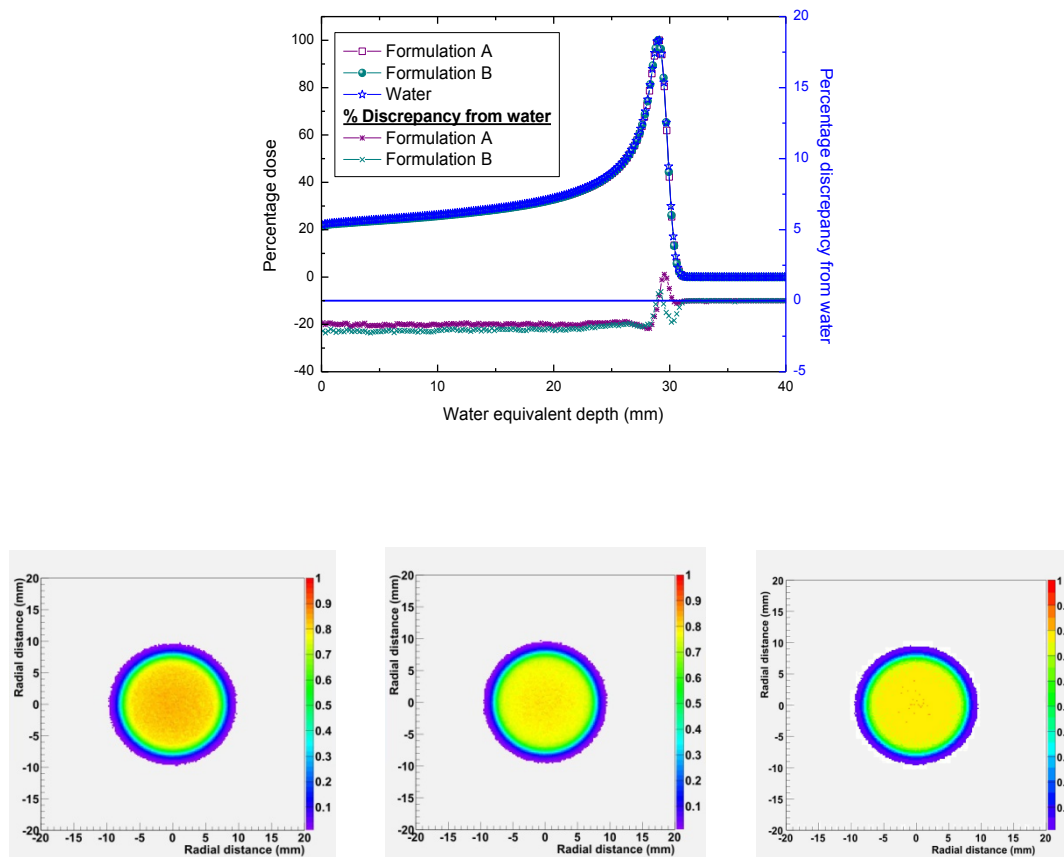
Figure 3: Top panel: Monte Carlo calculated total percentage dose versus water-equivalent depth for two PRESAGE® formulations and water. The discrepancy from water is plotted below and the scale is shown on the right axis. Bottom panel: Monte Carlo calculated cross-sectional total dose distributions normalized to dose at the Bragg peak calculated at 29.5 mm water equivalent depth for water, PRESAGE® formulation A and formulation B (left, middle and right, respectively).

5. References

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