Study of dosimetric water equivalency of PRESAGE® for megavoltage and kilovoltage x-ray beams

Tina Gorjiara¹, Robin Hill¹, Robin Hill², Jung-Ha Kim¹, Zdenka Kuncic¹, John Adamovics³, and Clive Baldock¹

¹ Institute of Medical Physics, School of Physics, University of Sydney, NSW 2006, Australia
² Department of Radiation Oncology, Royal Prince Alfred Hospital, Sydney, NSW 2050, Australia
³ Department of Chemistry and Biology, Rider University, Lawrenceville, NJ 08648, USA

clive.baldock@sydney.edu.au

Abstract. PRESAGE is a dosimeter that is suitable for 3D dosimetry. To be used as an ideal dosimeter, however, it should present radiologically water equivalent properties. In this work, we have investigated the radiological properties of three different PRESAGE® formulations. The radiological water equivalence was assessed by comparing the photon cross sections and radiation dosimetry properties of the three different PRESAGE® formulations with the corresponding values for water. Relative depth doses were calculated using Monte Carlo methods for 75, 125, 180 and 280 kVp and 6 MV x-ray beams. Based on the results of this study, the PRESAGE® formulations with lower halogen content are more dosimetrically water equivalent.

1. Introduction
The PRESAGE® dosimeter is composed of radiochromic components (leuco dyes) and halogen-containing free radical initiators that undergo a colour change after irradiating with ionizing radiation. As PRESAGE® is a three dimensional (3D) dosimeter, it has clinical application in modern radiation treatment techniques [1, 2].

To be used in radiation dosimetry, a 3D dosimeter should ideally be radiologically water equivalent [3]. The radiological properties of a material can be assessed by comparing the following parameters to the corresponding values for water: effective atomic number (Z_{eff}); mass energy absorption coefficient; mass stopping power; mass density (ρ); and electron density (ρ_e)[4-6].

The radiological properties of the original PRESAGE® formulation have been investigated previously [6]. It was found that the PRESAGE® formulation had an effective atomic number (Z_{eff}) that is 17% greater than that of water. Two subsequent PRESAGE® formulations have since been developed, with lower halogen content to potentially improve water equivalency over a larger energy range. In this work we have investigated and compared the radiological dosimetric properties and the water equivalency of the three PRESAGE® formulations. We calculated photon cross sections and mass energy absorption coefficients. We also determined depth doses in each of the dosimeters using Monte Carlo calculations for 6 MV and 75, 125, 180 and 280 kVp x-ray beams.
2. Materials and Methods

The elemental composition of each PRESAGE® formulation was calculated using their molecular formula and are summarized in Table 1. We henceforth refer to the lower halogen content PRESAGE® formulations as LHP1 and LHP2, and we refer to the original PRESAGE® formulation as OP. All three PRESAGE® formulations have been provided by the same manufacturer (Heuris Pharma, New Jersey, USA).

| Material                  | \( Z_{\text{eff}} \) | Formula                       | \( w_H \) | \( w_C \) | \( w_N \) | \( w_O \) | \( w_S \) | \( w_{Cl} \) | \( w_{Br} \) |
|--------------------------|----------------------|-------------------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| Lower halogen             |                      |                               |           |           |           |           |           |           |           |
| PRESAGE® 1 (LHP1)         | 7.688                | \( C_{1758}H_{3000}N_{122}O_{442}S_{4}Cl_{30}Br_{1} \) | 0.08850   | 0.6178    | 0.04960   | 0.2069    | 0.003800 | 0.03112   | 0.002300  |
| Lower halogen             |                      |                               |           |           |           |           |           |           |           |
| PRESAGE® 2 (LHP2)         | 7.740                | \( C_{1899}H_{1541}N_{60}O_{228}S_{10}Cl_{1}Br_{1} \) | 0.09050   | 0.6224    | 0.04899   | 0.2126    | 0.01870  | 0.002100  | 0.004700  |
| Original PRESAGE® (OP)    | 8.652                | \( C_{481}H_{842}N_{30}O_{129}Cl_{9}Br_{0} \) | 0.08920   | 0.6074    | 0.04460   | 0.2172    | -         | 0.03340   | 0.008400  |
| Water                     | 7.417                | \( H_2O \)                     | 0.1119    | -         | -         | 0.8881    | -         | -         |

Table 1: Effective atomic number, elemental composition, and fractional weight \( (w_k) \) for materials of interest.

Photon cross sections for photoelectric absorption, Compton scatter and pair production were obtained from the NIST XCOM database over the energy range 10 keV - 20 MeV [7]. The elemental data of mass energy absorption coefficients were taken from the NIST X-ray attenuation database and were calculated for each PRESAGE® formulation using the mixture rule and elemental compositions, and were then compared to those for water.

Depth dose calculations for the PRESAGE® dosimeters were performed using the EGSnrc/BEAMnrc Monte Carlo package (Version 4, Research Council of Canada, Ottawa, Canada) [8]. The phase space files for each of the x-ray beams were generated using the BEAMnrc user code. In all cases, the vendor geometric and material specifications were used in the modeling. The 6 MV x-ray beam was produced by a Varian 21iXs linear accelerator (Varian Medical Systems, city, state, USA). The beam was modeled with a field size of 10×10 cm² and the electron and photon energy cutoff parameters, ECUT and PCUT, were set to 0.7 MeV and 0.01 MeV, respectively. The kilovoltage x-ray beams were generated by a Pantak Therapax DXT300 kilovoltage x-ray therapy unit with a tube potential varying from 50 to 280 kVp using a previously published methodology [9]. For the kilovoltage Monte Carlo calculations, ECUT and PCUT were set to 0.521 MeV and 0.001 MeV, respectively.

We calculated depth dose curves in the three PRESAGE® formulations and water using the DOSRZnrc user code and phase space files generated by BEAMnrc for the 6 MV x-ray beam. Within DOSRZnrc, each phantom was defined as a cylinder. In the buildup region, the first 8 voxels were defined with 0.25 cm thickness and the next 16 voxels with 0.5 cm thickness [6]. For the kilovoltage x-ray beams, we calculated depth doses in a similar manner but using the DOSXYZnrc user code. Each phantom was defined in DOSXYZnrc with a total of 20 voxels of 0.5 cm thickness along the central axis.

For the comparison of the phantom materials, we determined the density thickness which is defined as the physical depth (cm) × density (g cm⁻²) [10].

3. Results

The calculated photon cross sections for the three different PRESAGE® formulations and water over the energy range 10 keV - 20 MeV are plotted in Figure 1. As indicated in Figure 1a, LHP1 and LHP2 exhibit significantly more water equivalent photoelectric absorption cross sections than OP. This may be attributed to a reduction in the proportion of bromine in the new PRESAGE® formulation compared to OP. LHP2 has the most water equivalent Compton scattering cross section. However, the pair production cross section of OP is closer to the value of water. This can be attributed to the pair
production cross section being approximately proportional to $Z^2/A$ at these energies and the highest fractional weighting is for oxygen in water, whereas it is for carbon in the PRESAGE® formulations.

Figure 1. Photon cross sections for (a) photoelectric absorption (b) Compton scattering and (c) pair production for the three PRESAGE® formulations and for water.

The ratio of the mass energy absorption coefficients of the PRESAGE® formulations and water are presented in Figure 2 for the photon energy range 10 keV - 20 MeV. A rapid increase in the relative mass energy absorption coefficient is noticeable over energies 10 - 40 keV, followed by a rapid decline towards 100 keV. At the peak, the mass energy absorption coefficient of OP is more than 75% higher than water, while the mass energy absorption coefficients of LHP1 and LHP2 are approximately only 20% higher than water.

Figure 2. The mass energy absorption ratio for LHP1, LHP2 and OP relative to water.
Figure 3 shows the Monte Carlo calculated depth doses for the three PRESAGE® formulations and water using a 6 MV x-ray beam. The depth doses are scaled according to the density thickness. The dose differences relative to the value of water are up to 2% for the lower halogen containing PRESAGE® formulations and up to 5% for OP at a radiological depth of 10 g cm\(^{-2}\).

**Figure 3.** Monte Carlo relative density corrected depth dose curves for a 6 MV x-ray beam for the three PRESAGE® formulations and for water.

Figure 4 shows the kilovoltage Monte Carlo calculated dose to density corrected depth for the PRESAGE® formulations and water. The depth dose curves suggest that the new PRESAGE® formulations LHP1 and LHP2 are more water equivalent than OP in terms of dose response. As the x-ray beam energy increases, the differences between the relative doses decreases, but the depth dose curves for the PRESAGE® formulations then begin to exhibit less attenuation than water for energies above 200 kVp. The changeover in relative depth dose curves from 180 kVp to 280 kVp can be attributed to the rapid decrease in the mass energy absorption coefficient at energies approaching 100 keV (see Figure 2), which is close to the mean energy of these beams.
4. Conclusion
These results indicate that the PRESAGE® formulations with lower halogen contents show more radiologically water equivalent properties than the original PRESAGE® formulation. The dose response of the lower halogen content PRESAGE® is comparable to the typical dose response of polymer gel dosimeters.

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