

Monte Carlo-based investigation of water-equivalence of solid phantoms at ^{137}Cs energy

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ABSTRACT

Investigation of solid phantom materials such as solid water, virtual water, plastic water, RW1, polystyrene, and polymethylmethacrylate (PMMA) for their equivalence to liquid water at ^{137}Cs energy (photon energy of 662 keV) under full scatter conditions is carried out using the EGSnrc Monte Carlo code system. Monte Carlo-based EGSnrc code system was used in the work to calculate distance-dependent phantom scatter corrections. The study also includes separation of primary and scattered dose components. Monte Carlo simulations are carried out using primary particle histories up to 5×10^9 to attain less than 0.3% statistical uncertainties in the estimation of dose. Water equivalence of various solid phantoms such as solid water, virtual water, RW1, PMMA, polystyrene, and plastic water materials are investigated at ^{137}Cs energy under full scatter conditions. The investigation reveals that solid water, virtual water, and RW1 phantoms are water equivalent up to 15 cm from the source. Phantom materials such as plastic water, PMMA, and polystyrene phantom materials are water equivalent up to 10 cm. At 15 cm from the source, the phantom scatter corrections are 1.035, 1.050, and 0.949 for the phantoms PMMA, plastic water, and polystyrene, respectively.

Key words: Brachytherapy; Monte Carlo simulations; solid phantom

Introduction

Brachytherapy refers to a method of treatment in which sealed radioactive sources are used to deliver radiation at short distances by interstitial, intracavitary, or surface mould applications. Brachytherapy delivers a high dose in the tumor and an acceptable low dose to surrounding normal tissue due to rapid dose fall-off with distance. American Association of Physicists in Medicine (AAPM) Task Group reports, AAPM TG43^[1] and TG43U1^[2] recommend

water as a reference medium for dosimetry of interstitial brachytherapy sources. Due to high dose gradients near brachytherapy sources and specification of the dose parameters within few centimetres of the source, source-detector distance should be specified very accurately for dosimetric measurements. Precise positioning of detectors, reproducibility of source and detectors in reference liquid water medium, and water proofing of detectors poses a practical problem. Solid phantom materials can be easily machined, to accommodate the source and detectors in a precise geometrical configuration, facilitating an accurate measurement and reproducibility in source-detector geometry.

Suitable solid phantom material should be selected to mimic the absorption and scattering of radiation as that in liquid water.^[3] Constantinou *et al.*,^[4] had studied the radiation characteristic of solid water, polystyrene, and lucite [polymethylmethacrylate (PMMA)] in the energy range 0.01-100 MeV for radiotherapy x-ray and gamma ray beam calibration and found that solid water is superior to the polystyrene and lucite phantom materials. Sahoo *et al.*,^[5] investigated water equivalence of various solid phantom materials for ^{60}Co brachytherapy source using the Monte Carlo methods. The authors concluded that the phantom materials RW1 and solid water represent water equivalent up to 20 cm from the source. Whereas, PMMA

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and polystyrene are water equivalent up to 10 and 15 cm from the source, respectively.

Meli *et al.*,^[6] studied dosimetric characteristics of solid water, polystyrene, and PMMA phantom materials using experimental and Monte Carlo methods in a bounded phantom material for ¹⁹²Ir brachytherapy source. The authors concluded that, under full scatter conditions, PMMA, polystyrene, and solid water are equivalent to water up to 10 cm distance. They also concluded that PMMA is not a suitable phantom material in the absence of full scatter, whereas polystyrene and solid water are suitable phantom materials even in the absence of full scatter. Tedgren and Carlsson^[7] also studied the influence of PMMA, solid water, and polystyrene phantom material and dimensions on ¹⁹²Ir source dosimetry. The authors concluded that water equivalence at a specified distance from the source depends not only on the size of the plastic phantom but also on the size of the water phantom used for comparison. Compared to equally sized water phantoms, polystyrene is less water equivalent than PMMA and solid water, but compared to larger water phantoms, polystyrene is most water equivalent. Water equivalence of solid phantom materials for ¹²⁵I brachytherapy source was studied by Meigooni *et al.*^[8] Dosimetric study for solid phantom material for ¹²⁵I and ¹⁰³Pd energies was studied by Meigooni *et al.*,^[9] Luxton,^[10] and Reniers *et al.*^[11]

To our knowledge, limited information is available on phantom scatter corrections at the ¹³⁷Cs energy. The study by Pérez-Calatyud *et al.*,^[12] is only limited to comparison of Monte Carlo-based dose distributions in a PMMA phantom to thermoluminescent dosimeter TLD-based measurements in a PMMA phantom. Meigooni *et al.*,^[13] studied the dosimetric properties of plastic water and solid water for photon energies in the range 20 keV-⁶⁰Co including 662 keV using the Monte Carlo methods. The

authors presented ratio of dose rate in medium to water only up to a distance of 5 cm for 662 keV photons.

The objective of the present study is to examine water equivalence of several solid phantom materials such as solid waterTM (Gammex- RMI, USA), virtual waterTM (MED-CAL, Inc., Wisconsin, USA), plastic waterTM (Computerized Imaging Reference Systems, Inc., Virginia, USA), PMMA, polystyrene, and RW1TM (PTW-Freiburg)^[13] at the ¹³⁷Cs energy. The study also includes separation of primary and scatter components of absorbed dose to water. We have used EGSnrc-based Monte Carlo system for this purpose.^[14]

Materials and Methods

Phantom materials

The atomic composition and density of the investigated phantom materials are given in Table 1. The electron density (ρ_e) of a phantom material was calculated from its mass density (ρ_m) and atomic composition according to equation 1 as presented by Shrimpton in his publication^[15] as below:

$$\rho_e = \rho_m \cdot N_A \cdot \left\langle \frac{Z}{A} \right\rangle \quad \dots(1)$$

where, $\left\langle \frac{Z}{A} \right\rangle = \sum_i a_i \left(\frac{Z_i}{A_i} \right)$, N_A is Avogadro's number and a_i is the fraction by weight of the i^{th} element of atomic number Z_i and Atomic weight A_i . The effective atomic number (Z_{eff}) is the atomic number of an element with which photons interact the same way as with the given composite material. Mayneord^[16] has defined Z_{eff} of a compound as given below in expression (2) and here Z_{eff} is considered for photoelectric interaction.

$$Z_{\text{eff}} = (a_1 Z_1^{2.94} + a_2 Z_2^{2.94} + a_3 Z_3^{2.94} + \dots + a_n Z_n^{2.94})^{1/2} \quad \dots(2)$$

Table 1: Elemental composition, mass fraction, mass density, $\langle Z/A \rangle$, and average atomic number of water and solid phantom materials

Element	Z	A	Water ¹	Solid water ²	RW1 ²	Plastic water ³	Virtual water ⁴	PMMA ¹	Polystyrene ¹	
Composition and mass fraction	H	1	1.008	0.1119	0.081	0.132	0.093	0.077	0.08054	0.07742
	C	6	12.01		0.672	0.794	0.6282	0.687	0.59985	0.92258
	N	7	14.01		0.024		0.010	0.023		
	O	8	15.99	0.8881	0.199	0.038	0.1794	0.189	0.31961	
	Mg	12	24.31			0.009				
	Cl	17	35.46		0.001	0.027	0.0096	0.001		
	Ca	20	40.08		0.023		0.0795	0.023		
Br	35	79.90				0.0003				
Mass density (g/cm ³)			1.000	1.036	0.970	1.013	1.030	1.190	1.060	
$\langle Z/A \rangle$			0.555	0.540	0.565	0.545	0.538	0.539	0.538	
$Z_{\text{Effective}}$			7.42	7.38	7.14	9.37	7.38	6.47	5.70	

¹Adapted from Hubbell and Seltzer^[17], ²Adapted from ICRU-44^[13], ³Adapted from Meigooni *et al.*^[13], ⁴Adapted from Reniers *et al.*^[11] PMMA: Polymethylmethacrylate

Where, $a_1, a_2, a_3, \dots, a_n$ are the fractional contributions of each element to the total number of electrons in the mixture. Z_1, Z_2, \dots, Z_n are the atomic number of each element.

The elemental composition of phantom materials for Monte Carlo simulation should be considered carefully. Meigooni *et al.*,^[9] have indicated that the discrepancies in phantom material composition can significantly affect the conversion factors estimated for water equivalent phantom materials used in low energy brachytherapy sources. In present study, the atomic composition and density of solid water was adapted from the work of Meigooni *et al.*^[9] The composition and density of water, PMMA, and polystyrene are adapted from work of Hubbell and Seltzer.^[17] Similarly, the composition and density details of RW1, plastic water, and virtual water are adapted from ICRU-44³, Meigooni *et al.*,^[13] and Reniers *et al.*,^[11] respectively. Table 2 presents the values of linear attenuation coefficient and mean-free path in different phantom materials at ¹³⁷Cs energy (0.662 MeV). These data are adapted from Hubbell and Seltzer compilations.^[17]

Analysis of photon interaction cross-section

Figure 1 shows the ratio of mass attenuation coefficient of solid phantom materials to that of liquid water, $(\mu/\rho)_{\text{Phant}}/(\mu/\rho)_{\text{Wat}}$ as a function of photon energy, where the suffice “Phant” refers to phantom material other than water. The values of mass attenuation coefficient of solid water, virtual water, and RW1 are comparable to that of water for photons in the energy range 15 keV-1.5 MeV (maximum deviation

is less than about 3%). For PMMA and polystyrene, for photon energies less than 100 keV, $(\mu/\rho)_{\text{Phant}}$ value is less compared with $(\mu/\rho)_{\text{Water}}$. For plastic water, the $(\mu/\rho)_{\text{Phant}}$ value is significantly higher than that of water for photon energies below 100 keV. Above 100 keV, the $(\mu/\rho)_{\text{Phant}}$ values of PMMA, polystyrene and plastic water are comparable within 3% when compared with that of liquid water.

Contribution of photoelectric effect and Compton scattering (CS) to total mass attenuation coefficient was studied by using the state-of-the art XCOM^[18] photon interaction data set. The ratio of photoelectric cross-section to the total cross-section of the phantom material $(\sigma_{\text{PE, Phant}}/\sigma_{\text{Tot, Phant}})$ is presented in Figure 2. As seen from the figure, the ratio $\sigma_{\text{PE, Phant}}/\sigma_{\text{Tot, Phant}}$ for photons in the energy range 10-200 keV in solid water, virtual water, and RW1 is comparable to that of water. In phantom material having smaller Z_{eff} such as polystyrene ($Z_{\text{eff}} = 5.70$) and PMMA ($Z_{\text{eff}} = 6.47$) as compared with water ($Z_{\text{eff}} = 7.42$), the contribution of photoelectric effect to total interaction cross-section in material is less than that of water. Whereas, for the materials with Z_{eff} values more than that of water, such as Plastic Water ($Z_{\text{eff}} = 9.37$), larger contribution of photoelectric effect to the total cross-section of the phantom material is observed.

The ratio of CS cross-section to the total cross-section of phantom material $(\sigma_{\text{CS, Phant}}/\sigma_{\text{Tot, Phant}})$ as a function of photon energy is shown in Figure 3. This ratio for Solid Water, Virtual Water and RW1 are comparable to that of water. Polystyrene and PMMA show more contribution of

Table 2: Linear attenuation coefficient μ (cm⁻¹) and mean free path τ (cm) of 0.662 MeV photon for water and solid phantom materials

μ or τ	Water	Solid water	RW1	Plastic water	Virtual water	PMMA	Polystyrene
μ	0.0857	0.0888	0.0845	0.0853	0.0855	0.0990	0.0879
τ	11.67	11.26	11.83	11.72	11.70	10.10	11.38

PMMA: Polymethylmethacrylate

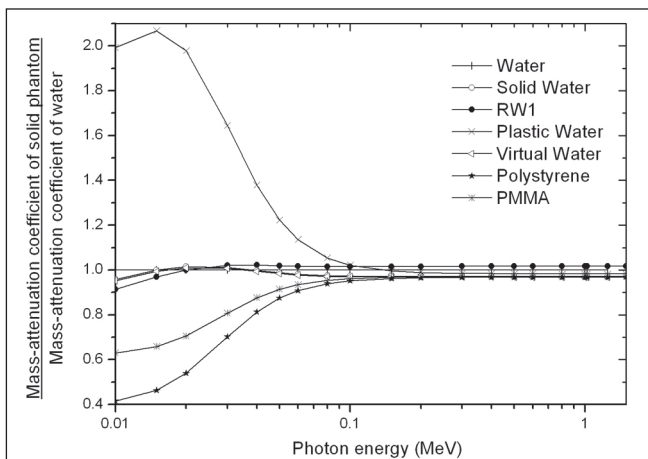


Figure 1: Ratio of mass-attenuation coefficient of solid phantoms to liquid water presented as a function of photon energy

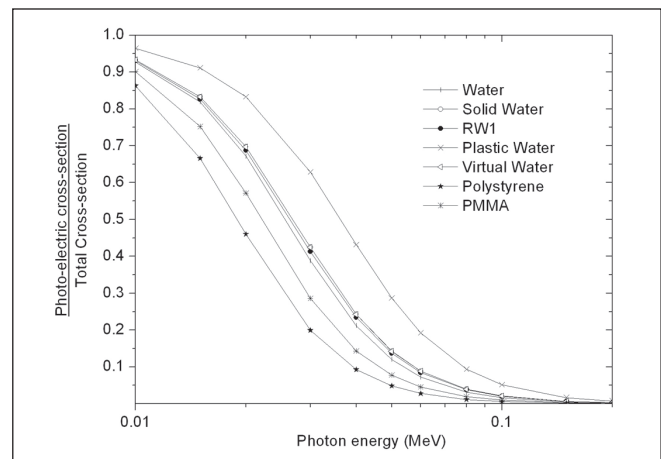


Figure 2: Ratio of photoelectric cross-section to total cross-section presented for water and solid phantoms as a function of photon energy

CS to the total cross-section as compared to that of water. For plastic water, the contribution of CS to total cross-section is less than that of water for photon energies less than 200 keV.

Monte Carlo calculations

In the Monte Carlo calculations, the absorbed dose to water is scored for radial distances $r = 1-15$ cm in the liquid water and solid phantom materials in spherical shells of thickness 0.1 mm using the EGSnrcMP-based^[14] EDKnr^[19] user code. In the case of solid phantom materials, the 0.1 mm thick spherical scoring region was filled with water. The radius of the material phantom is 50 cm, which provides full scatter up to 20 cm. This approach is based on the study of Granero *et al.*,^[20] on the impact of phantom size and shape in brachytherapy dosimetry and Pérez-Calatayud *et al.*,^[21] that a spherical phantom 40 cm in radius mimics an unbounded phantom for ¹³⁷Cs for full scatter conditions within 1% for distances less than 20 cm from the source. The density of water considered is 0.998 g/cm³ at 22°C.^[2] For Monte Carlo calculations, we have considered only 662 keV gamma energy of ¹³⁷Cs emission (yield of 662 keV: 0.851 photon/disintegration).^[22] In the Monte Carlo calculations, we ignored x-rays from ¹³⁷Ba, as in a previously published study by Selvam *et al.*,^[23] it was demonstrated that these x-rays were not important.

We have also calculated phantom scatter corrections for the PMMA phantom for the commercial ¹³⁷Cs source of Radiation Therapy Resources Inc., Valencia, CA (RTR)^[24] to compare with the point source-based phantom corrections. For simulation of ¹³⁷Cs RTR brachytherapy source, we have used the FLURZnr^[19] user code. The phantom dimensions considered are 50 cm diameter × 50 cm height. In the calculations photon fluence spectrum was initially scored which was subsequently converted to water-kerma by using the mass-energy-absorption coefficients of water from Hubbell and Setlzer.^[17]

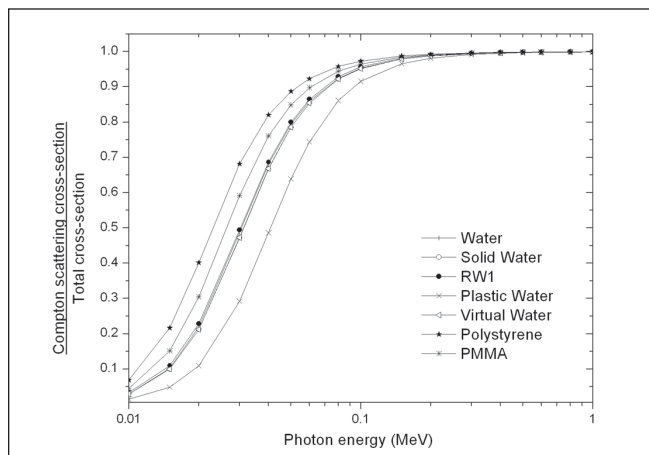


Figure 3: Ratio of Compton scattering cross-section to total cross-section presented for water and solid phantoms as a function of photon energy

Monte Carlo parameters and statistical uncertainties

The PEGS4 data set needed for the Monte Carlo calculations is based on widely used XCOM compilations.^[18] The low-energy threshold for the production of knock-on electrons (AE) is set to 521 keV for an electron with 10 keV kinetic energy, and the threshold for secondary bremsstrahlung photons (AP) is set to 10 keV.

All Monte Carlo simulations utilized the PRESTA-II electron step length and EXACT boundary-crossing algorithms. The electron step size parameter, ESTEP is set to 0.25. To increase the speed of the calculations, for all simulations, electron range rejection technique is used by setting ESAVE = 2 MeV. The value of photon transport cutoff parameter PCUT used in all simulations is 10 keV. The value of ECUT used in EDKnr and FLURZnr calculations is 2 MeV. This means detailed electron transport is not necessary as water-kerma may be approximated to absorbed dose at ¹³⁷Cs energy.

Up to 5×10^9 primary photon histories are simulated. The statistical uncertainties on the calculated estimates have a coverage factor $k = 1$. Uncertainties on the dose values from the EDKnr simulations are less than 0.3%.

Results and Discussion

Reference dose rates

Table 3 compares dose rate per unit activity (cGy h⁻¹ mCi⁻¹) in liquid water phantom at 1 cm from the ¹³⁷Cs point isotropic source calculated in the present study against Melhus and Rivard.^[25] The dose rate values calculated by including Barium x-rays compare well.

Analysis of dose components

The primary component of water-kerma at a radial distance r (in Gy/photon) due to a monoenergetic point photon source is given by:

$$D_p(r) = \frac{k}{4\pi r^2} \cdot e^{-\mu_{\text{phant}}(E) \cdot r} \cdot E \cdot \left[\frac{\mu_{\text{en}}}{\rho}(E) \right] \quad \dots(3)$$

where, k is the unit conversion constant from MeV/g to J/kg, $\mu_{\text{phant}}(E)$ is the linear attenuation coefficient of the phantom material at photon energy E , and $[\mu_{\text{en}}/\rho(E)]_w$ is mass-energy-absorption-coefficient of water at E . For ¹³⁷Cs source, $E = 0.662$ MeV.

Table 3: Dose rate per unit activity (cGy h⁻¹ mCi⁻¹) in the liquid water phantom at 1 cm for the ¹³⁷Cs point source

Present study	Melhus and Rivard ^[25]
3.085 ^a	–
3.148 ^b	3.153 ^b

^afor single photon energy of 0.662 MeV, ^bas per NUDAT spectrum including Barium X-rays^[22]

Figure 4 presents the ratio of primary component of water-kerma in a solid phantom material to that in liquid water as a function of r from the ^{137}Cs point source (calculated using equation (3)). Deviation of this ratio from unity is due to differences in the values of linear attenuation coefficients of the phantom materials (difference is up to 18% at 15 cm for PMMA).

The scatter component of the absorbed dose, $D_s(r)$ was obtained by subtracting $D_p(r)$ from the EDKnr-calculated total dose. The scatter-to-primary ratio $D_s(r)/D_p(r)$ helps in understanding the differences in the scattering of photons in different phantom materials. This ratio is plotted in Figure 5 for the investigated phantom materials. Although the absolute values of $D_s(r)$ decrease with r , the ratio $D_s(r)/D_p(r)$ increases because of the inverse square fall of $D_p(r)$. Table 4 presents the distance at which $D_s(r)$ equals $D_p(r)$ for the investigated phantom materials. Figure 6 presents dose per unit energy multiplied by $4\pi r^2$ per source photon as a function of r from the ^{137}Cs point source.

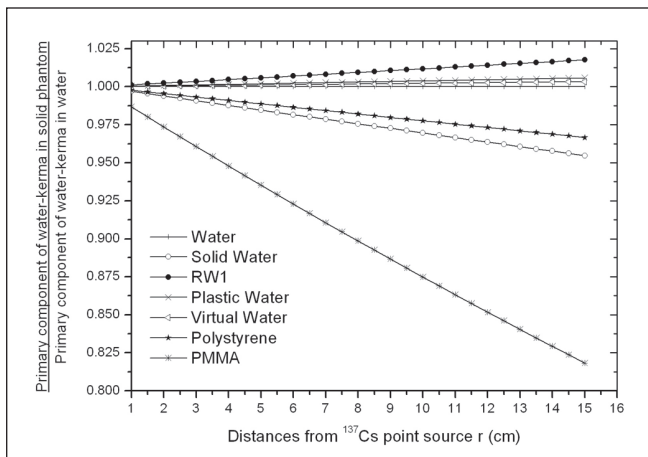


Figure 4: Ratio of primary component of dose in solid phantoms to that in liquid water phantom presented as a function of radial distance r from ^{137}Cs point source

Phantom scatter correction factor

The measurement-based absorbed dose to water in solid water phantoms is required to be corrected for differences in attenuation and scattering between solid phantom materials and liquid water to obtain absorbed dose to water in liquid water phantom. The distance-dependent phantom scatter correction $K(r)$ is given below:

$$K(r) = \frac{\text{Dose to water at distance } r \text{ in liquid water}}{\text{Dose to water at distance } r \text{ in solid phantom material}} \dots (4)$$

Table 5 presents the values of $K(r)$ for select distances of $r = 5 \text{ cm}, 10 \text{ cm},$ and 15 cm from the source in solid phantom materials. The statistical uncertainty in the calculated phantom scatter corrections is less than 0.4%. The values of $K(r)$ calculated for PMMA phantom based on the point source compare within 0.5% with that of the ^{137}Cs RTR brachytherapy for distances up to 15 cm from the source. Figure 7 represents phantom scatter correction $K(r)$ for solid phantoms as a function of radial distance r from ^{137}Cs point source. At 5 cm from the source, all the investigated phantoms are water-equivalent. This observation is

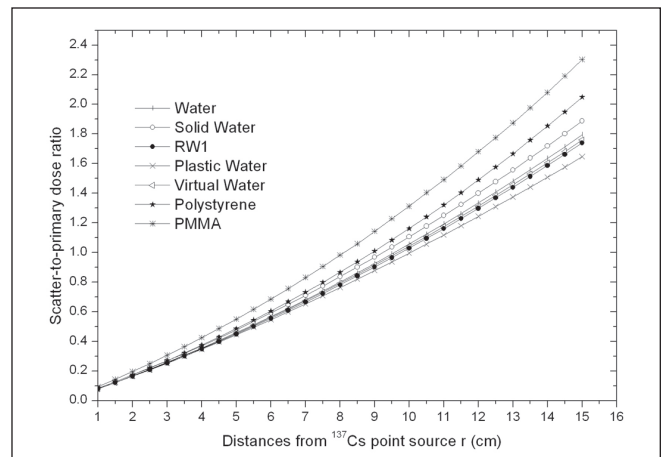


Figure 5: Ratio of scatter-to-primary component of absorbed dose in water and solid phantoms as a function of radial distance r from ^{137}Cs point source

Table 4: Distance (in cm) from the ^{137}Cs point source at which scatter to primary ratio, $D_s(r)/D_p(r)$ is unity for water and solid phantom materials

Water	Solid water	RW1	Plastic water	Virtual water	PMMA	Polystyrene
10.0	9.5	10.0	10.5	10.0	8.5	9.0

PMMA: Polymethylmethacrylate

Table 5: Phantom scatter corrections for solid phantom materials at distances of 5, 10, and 15 cm from the ^{137}Cs point source

Distance (cm)	Solid water	RW1	Plastic water	Virtual water	PMMA	Polystyrene
5	1.0021	1.0002	1.0079	1.0015	1.0064	0.9925
10	1.0070	1.0017	1.0264	1.0048	1.0168	0.9732
15	1.0139	1.0029	1.0502	1.0095	1.0346	0.9485

PMMA: Polymethylmethacrylate

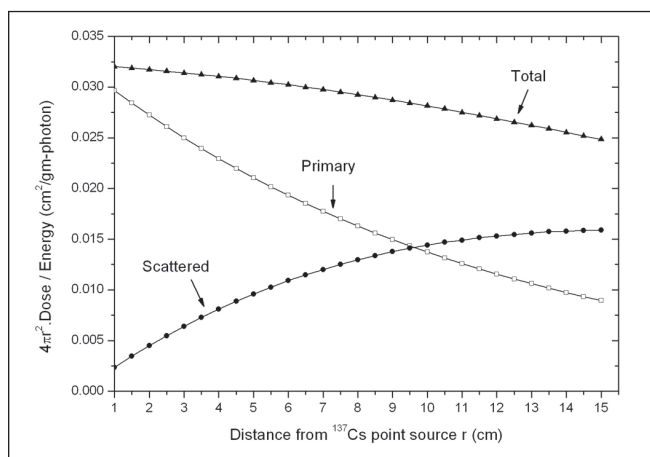


Figure 6: The dependence of primary, scattered, and total dose in water multiplied by $4\pi r^2$ per unit mean energy versus radial distance r from ^{137}Cs point source in water

consistent with the study carried by Meigooni, *et al.*,^[13] for the solid water and plastic water phantoms. Solid water, virtual water, and RW1 are suitable phantom materials for the dosimetry up to a distance of 15 cm from the source. Phantom materials such as plastic water, PMMA and polystyrene phantom materials are water-equivalent for distances up to 10 cm. At 15 cm, the phantom scatter corrections are 1.035, 1.050, and 0.949 for the phantoms PMMA, plastic water, and polystyrene, respectively.

Conclusion

Water equivalence of solid phantoms such as solid water, virtual water, RW1, PMMA, polystyrene, and plastic water materials are investigated at ^{137}Cs energy for distances up to 15 cm from the source. The Monte Carlo-based investigation suggests that the phantom materials such as virtual water, RW1, and solid water are water equivalent up to 15 cm from the source. Polystyrene phantom demonstrates that the corrections are always smaller than unity and the deviation from unity is larger as the distance from the source increases. For example, the corrections at 10 and 15 cm for this phantom are about 2.5% and 5% smaller than unity, respectively. For PMMA phantom the phantom scatter correction is less 1% for distances up to 8 cm and it increases to about 3.4% at 15 cm. The corrections for the plastic phantom are about 2.5% and 5% larger than unity at distances 10 and 15 cm, respectively. The corrections obtained for the phantoms virtual water and solid water are comparable at all distances. The investigation demonstrates the importance of evaluation of water equivalence of a solid phantom material prior to its use in dosimetric measurements.

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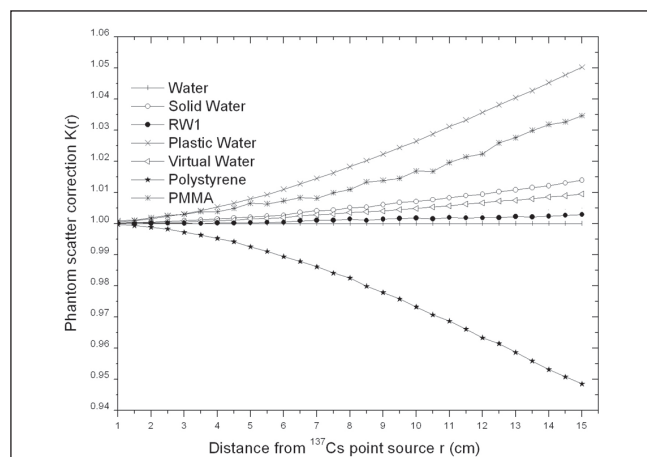


Figure 7: The phantom scatter correction $K(r)$ for solid phantoms as a function of radial distance r from ^{137}Cs point source

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