Radiological Properties of Selective Monomers of Polymer Gel Dosimeter in Radiotherapy Application

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The goal of this study is to calculate the electron density, effective atomic number, mass attenuation and mass energy absorption co-efficient and kinetic energy released per unit mass for five different monomers, which are used in the polymer gel dosimeter in radiotherapy application. Power law method and Auto-Z_{eff} software were used to calculate the effective atomic number. National Institute of Standard and Technology (NIST) database was used to calculate mass attenuation and energy absorption coefficient. Electron density of the acrylamide was higher ($3.40E + 23$ e/cm^3) than other monomers and N-isopropyal acrylamide has least electron density ($2.76E + 23$ e/cm^3). Each monomer has an identical effective atomic number over the energy range from 0.01 to 20 MeV. The rapid fall occurred in the kinetic energy released per unit mass at low energy. At low energy region kinetic energy released per unit mass of acrylic acid was higher than others and it was opposite in higher energy region. The behaviour of kinetic energy released per unit mass and effective atomic number similar with function of energy. Effective atomic number of *n*-vinyalpyrrolidine has good agreement with water (0.003 % discrepancy).

Keywords: Effective atomic number, Electron density, Polymer gel, monomer.

INTRODUCTION

The understanding of the interaction of radiation with matter is an essential part in the field of nuclear physics, nuclear engineering, medical physics, radiation protection, radio-biology and health physics. In medical physics, dosimetry is the major part of the system, which can be used to measure the radiation dose. To measure the dose different types of detectors are available such as ion chambers, diodes, films and thermo luminescence dosimeter (TLD). The mentioned dosimeters are measuring the dose in 1 and 2 dimensionally. But in modern radiotherapy, measurements of dose in 3*d* are a supreme procedure. Gel dosimeter is an excellent system to measure the radiation dose in 3*d* [1] and it has various characteristics such as tissue equivalents, energy independent, less dose rate dependent, angular independent for incident photon beam and act as the phantom as well as detector so there is no space for the word of fluency perturbation correction factor [2]. Gel dosimeter comes under the chemical dosimeter which is divided into two parts, one is Fricke gel dosimeter (an inorganic gel dosimeter) and another one is polymer gel dosimeter (an organic gel dosimeter). Fricke gel contains ferrous ammonium solution, gelatin, sulfuric acid, water and ion indicators. Upon irradiation of ionizing radiation ferrous ions converted into

ferric ions and these conversions quantified by nuclear magnetic resonance and the absorption spectroscopy [3,4]. The major drawback of the Fricke is the diffusion of (ferric) ions from their origin and make it less reliable dose estimation [5]. A polymer gel dosimeter is fabricated mainly by, gelatin, water and different radio sensitive monomers such as acrylamide [6,7], methaacrylic acid (MAA) [8,9], N-isopropylacrylamide (NIPAM) [10,11], *n*-vinylpyrolidine (*n*-VPL) [12,13], 2-hydroxyethyl methacrylate (HEMA) [14,15] and acrylic acid [16,17]. Upon irradiation of ionizing radiation monomers will be converted into a polymer hence it is called polymer gel dosimeter. The conversion of monomers can be quantified to measure the absorbed dose using different techniques such as MRI, optical CT, X-ray CT and UV-visible absorption spectrophotometer [18-21]. Any material which is adopted in the dosimetry, it should be evaluated by its radiological properties such as, electron density and effective atomic number mass attenuation coefficient, mass energy absorption coefficient. In the present study radiological evaluation performed on the monomers which are used in the polymer gel dosimeter. Hence monomers are building blocks of polymer gel it is necessary to evaluate the radiological properties. Table-1 shows the molecular formula and the mass density of the monomers.

TABLE-1
MOLECULAR FORMULA AND DENSITY OF MONOMERS

Monomers	m.f.	Density (g/cm³)
Acrylamide	C_3H_5NO	1.130
Methaacrylic acid	$C_4H_6O_2$	1.020
N-Isopropylacrylamide	$C_6H_{11}NO$	0.915
n-Vinylpyrrolidine	C_6H_9NO	1.040
2-Hydroxyethyl methacrylate	$C_6H_{10}O_3$	1.070
Acrylic acid	$C_3H_4O_2$	1.050

EXPERIMENTAL

Effective atomic number and electron density: The interaction of the photons with any compound depends on their effective atomic number (Z_{eff}) and electron density (ρ_e). So it is very important to calculate Z_{eff} and ρ_e for the monomers. Z_{eff} can be calculated from the following equation [22].

$$Z_{eff} = (a_1 Z_1^{2.94} + a_2 Z_2^{2.94} + \dots\dots a_n Z_n^{2.94})^{1/2.94} \qquad (1)$$

where $a_1, a_2, a_{3\dots} a_n$ are the fractional contribution of each element in the given compound. Single value for Z_{eff} may not be adequate for compound materials over a range of energies [23], we used Auto-Z_{eff} software [24] for calculating the Z_{eff} from 0.01 to 20 MeV. The electron density is given by the following equation:

$$\rho_e = \rho.N_A.\Sigma_i w_i \left(\frac{Z_i}{A_i}\right) \qquad (2)$$

where ρ_e is the electron density, ρ is the mass density of the compound, N_A is the Avagadro's number, w_1 is the fraction by mass of the ith element of atomic number Z_i and atomic mass A_i [23].

Mass attenuation coefficient (μ/ρ) and mass energy absorption coefficient (μ_e/ρ): Mass attenuation coefficient (μ/ρ) is the measure of the average number of interactions between incident photon and matter that occur in a given mass-per-unit area thickness of the material [25]. Most of the electrons set in motion by photons will spend their energy by inelastic collision, but few electrons interact with the nucleus and will lose their energy in terms of bremsstrahlung X-ray photons and these photons are radiated out of the volume of interest and it is not included in the absorbed dose calculation in the volume of interest. Mass energy absorption coefficient can be used to account these kind of radiation loss and it is a very important quantity in dosimetry to quantify the absorbed radiation dose [22]. Mass attenuation and mass energy absorption coefficient of each element (H, C, N and O) was taken from the literature [26] and sum these values of the elements present in monomers to get the coefficient. It is given by the following equations:

$$(\mu/\rho)_{monomer} = \Sigma_i w_i (\mu/\rho)_i \qquad (3)$$

$$(\mu_{en}/\rho)_{monomer} = \Sigma_i w_i (\mu_{en}/\rho)_i \qquad (4)$$

where $(\mu/\rho)_{monomer}$ is the mass attenuation coefficient of monomer, w_i is fraction by mass of ith element, $(\mu/\rho)_i$ is the mass attenuation coefficient of ith element of the monomer, μ_{en}/ρ is the mass energy absorption coefficient of monomer and $(\mu_{en}/\rho)_i$ is the mass energy absorption coefficient of ith element of the monomer.

Kinetic energy released per unit mass (KERMA): Kinetic energy released per unit mass is defined as the sum of the initial kinetic energy of all the charged particles liberated by an uncharged particle in a unit mass of the material [22]. Kinetic energy released per unit mass relative to air for the monomers were calculated by the following equation:

$$K_a = \left(\frac{K_{monomer}}{K_{Air}}\right) = \frac{(\mu_{en}/\rho)_{monomer}}{(\mu_{en}/\rho)_{Air}} \qquad (5)$$

where $(\mu_{en}/\rho)_{monomer}$ is the mass energy absorption coefficient of the monomer and $(\mu_{en}/\rho)_{Air}$ is the mass energy absorption coefficient of air.

RESULTS AND DISCUSSION

Effective atomic number and electron density: Table-2 shows the elemental composition (% weight fraction), electron density and effective atomic numbers of different monomers.

The electron density of the acrylamide was higher than others because it have a higher mass density (1.13 g/cm³) and N-isopropylacrylamide has a least electron density of in the group due to less mass density (0.915 g/cm³). Fig. 1 shows the strong co-relation between mass and electron density. Effective atomic number of the *n*-vinylpyrrolidine is superior (7.44) to other monomers and it is very close to water (7.417) [27] with 0.003 % discrepancy. The effective atomic number (Z_{eff}) of 2-hydroxyethyl methacrylate has 22.03 % discrepancy from water. The effective atomic number is varied with respect to energy of incident photons hence it was calculated for the energy range of 0.01 to 20 MeV. Auto - Z_{eff} software was used to perform this calculation.
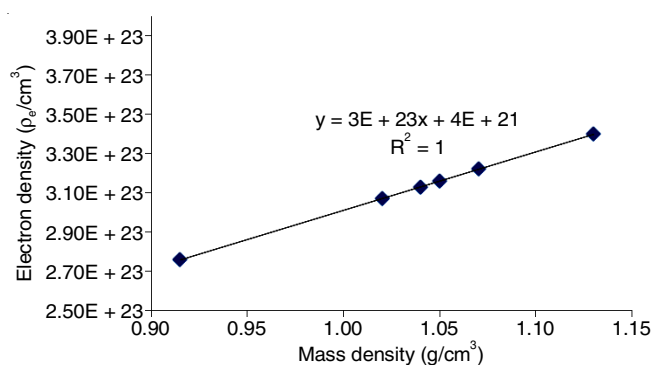

Fig. 1. Relation between electron density and mass density of monomers

TABLE-2
ELEMENTAL COMPOSITION (% WEIGHT FRACTION) AND ELECTRON DENSITY (ρ_e/cm^3)

Monomers	WH	WC	WO	WN	(ρ_e/cm^3)	Z_{eff}
Acrylamide	0.0709	0.506944	0.225094	0.197059	3.40E + 23	6.63
Methaacrylic acid	0.0703	0.558064	0.371688	–	3.07E + 23	6.77
N-Isopropylacrylamide	0.0980	0.636853	0.141388	0.123779	2.76E + 23	7.18
2-Hydroxyethyl methacrylate	0.0775	0.553742	0.368810	–	3.22E + 23	5.77
n-Vinylpyrrolidine	0.0816	0.648404	0.143953	0.126024	3.13E + 23	7.44
Acrylic acid	0.0560	0.500017	0.444036	–	3.16E + 23	5.97

Fig. 2 shows the Z_{eff} of all the monomers with function of energy. All monomers have different Z_{eff} because they have different proportion of hydrogen, oxygen, carbon and nitrogen and their mean atomic number also differ from each other (Table-3). All the monomers have maximum Z_{eff} in the energy range of 0.01 to 0.03 MeV. Among the monomers acrylic acid shows higher Z_{eff} at 0.01 MeV because it has highest mean atomic number. Since photoelectric absorption proportional to Z^4 of acrylic acid shows maximum (mean z = 4.2) and N-isopropylacrylamide (mean z = 3.4) shows minimum Z_{eff} at this energy range.
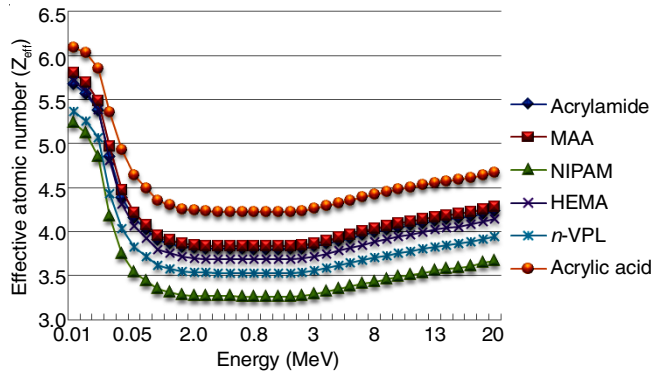

Fig. 2. Effective atomic number of monomers

TABLE-3
MEAN ATOMIC NUMBER OF MONOMERS

Monomers	Mean atomic number
Acrylamide	3.80
Methaacrylic acid	3.83
N-Isopropylacrylamide	3.44
n-Vinylpyrrolidine	3.53
2-Hydroxyethyl methacrylate	3.68
Acrylic acid	4.22

All other monomers fall into intermediate values of Z_{eff}. Beyond 0.03 MeV, Z_{eff} drops to a lower value up to 0.05 MeV because the typical Compton scattering begins. From 0.05 to 4 MeV all the monomers behave constantly, at this energy range Compton scattering is the predominant and it is proportional to the mean Z of the given compound. For a given monomer the minimum value of Z_{eff} found in this energy region (0.05 to 4 MeV). At this energy range all the monomers fall in their own mean Z region. From 1 to 1.25 MeV all monomers were fall into lower Z_{eff} except methaacrylic acid it was fall at 0.6 MeV. Since acrylamide, methaacrylic acid has almost same mean Z_{eff} (3.83 and 3.80) they behave very similar from 0.01 to 20 MeV. Beyond 5 MeV Z_{eff} increases with increasing energy as the pair production dominant interaction.

Mass attenuation co-efficient (μ/ρ) and mass energy absorption coefficient (μ_e/ρ): It is noted that μ/ρ of all the monomers decrease rapidly with increasing energy up to 0.01 MeV and decrease slowly up to 20 MeV (Figs. 3 and 4). The rapid fall of μ/ρ in the low energy range (0.001 to 0.01 MeV) is due to photoelectric absorption, where photon interaction cross-section depends on Z^3 for low energy [22].

Above 0.01 MeV Compton scattering is dominant than photoelectric absorption. Acrylic monomer has a maximum (μ/ρ) than others over the energy range from 0.01 to 20 MeV.
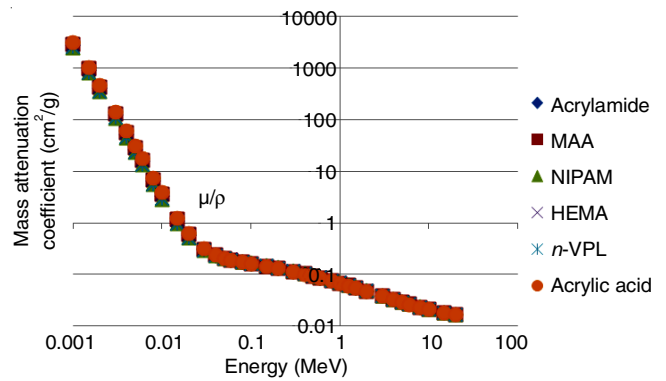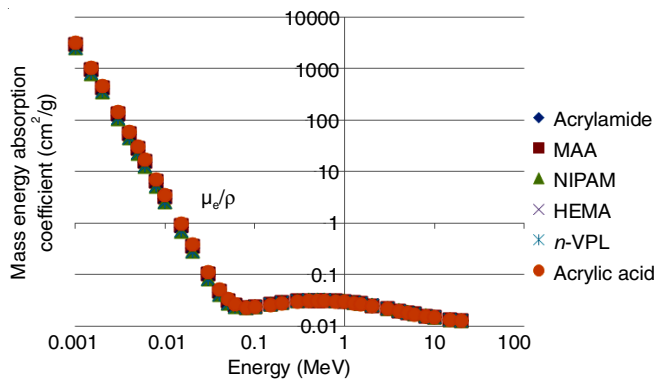

Fig. 3. Mass attenuation co-efficient of monomers

Fig. 4. Mass energy absorption co-efficient of monomers

It is because acrylic acid has a highest elemental composition of oxygen. Oxygen has highest (μ/ρ) (0.213 cm^2/g) than other elements presented in monomers such as H, C and N. (μ_e/ρ) decrease rapidly up to 0.03 MeV due to the dominate process of photoelectric absorption and beyond 0.03 MeV, it is decreasing slowly by Compton scattering replaces the photoelectric absorption.

Kinetic energy released per unit mass (KERMA): The KERMA relative to air (K_a) of the monomers plotted as a function of photon energy from 0.01 to 10 MeV in Fig. 5. The variation of the KERMA is similar to the variation of Z_{eff}. To show the similarities in their variations, two monomers were randomly selected and a plot was made for 0.01 to 0.05 MeV and 1 to 5 MeV [Fig. 6(a&b)].
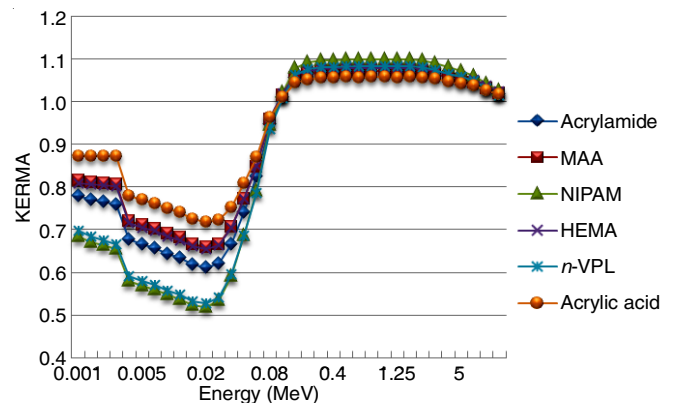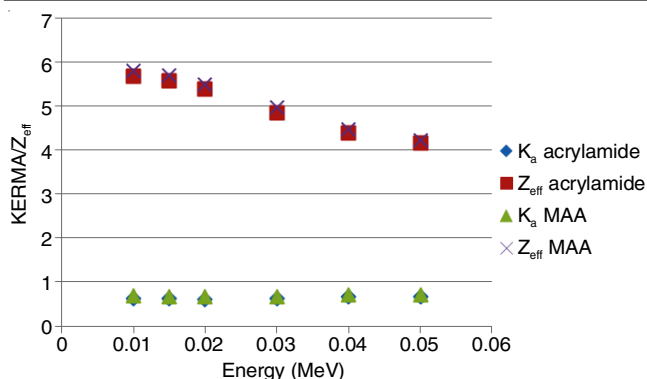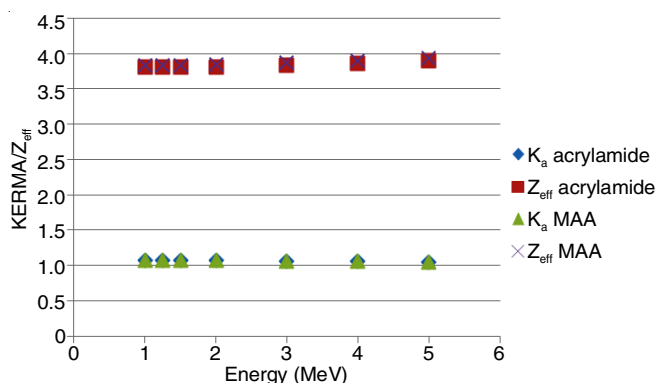

Fig. 5. KERMA of monomers

Fig. 6a. KERMA *vs.* Zeff at 0.01 to 0.05 MeV

Fig. 6b. KERMA *vs.* Z_{eff} at 1 to 5 MeV

From the figure it is well understood both KERMA and Z_{eff} behave in almost similar manner. The variations in the KERMA reflect the impacts of photon interaction process such as photoelectric absorption, Compton scattering and pair-production [28]. Acrylic acid has larger KERMA than other monomers and N-isopropylacrylamide is the least one at low energy region because of the major process of photoelectric absorption. In higher energy region 0.1 to 10 MeV, N-isopropyl-acrylamide has larger KERMA than acrylic acid due to the predominant process of compton scattering.

KERMA for all the monomers were constant in the energy range of 0.1 to 1.25 MeV. Throughout the energy range all monomers have intermediate KERMA values between acrylic acid and N-isopropylacrylamide.

Conclusions

• Electron density and energy dependent Z_{eff} was calculated for monomers used in the polymer gel dosimeter. As per the elemental composition each monomer has their identical Z_{eff} from 0.01 to 20 MeV. All the monomers have maximum Z_{eff} in the energy range of 0.01 to 0.03 MeV. Since acrylamide, methaacrylic acid has almost same mean Z (3.83 and 3.8) they behave very similar from 0.01 to 20 MeV.

• (μ/ρ) and (μ_e/ρ) were found larger values for acrylic acid and less for N-isopropylacrylamide this mainly due to proportion of high Z material presented in the given monomer. Acrylic acid has highest oxygen proportion and N-isopro-pyacrylamide has less proportion. (μ/ρ) of all the monomers were almost same from 0.05 to 20 MeV because of the Compton scattering it is independent of Z. Rapid fall of coefficient at low energy and slow follow at higher energy regions is impact of photoelectric absorption and Compton scattering, respectively.

• Kinetic energy released per unit mass relative to air was calculated and shown graphically. N-Isopropylacrylamide has less KERMA in low energy and it is opposite at high energy because of photo-electric absorption inversely proportional to E and Compton scattering replace the photo electric absorption at high energy. One should consider the properties of monomers before adapt in radiotherapy application.

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