RESEARCH ARTICLE

MEASUREMENT OF EFFECTIVE ATOMIC NUMBER AND ELECTRON DENSITY OF CARBOHYDRATES BY USING NIST, Geant4 AND NaI(Tl) : A COMPARATIVE STUDY.

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Manuscript Info	*Abstract*
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Introduction:-

The ionizing radiation effect on biological material such as amino acid, carbohydrates, lipids, fatty acids depends on the absorbed dose. Data on the transmission and absorption of gamma ray in biological, shielding and dosimetric materials assumes great significance by virtue their diverse application in the field of radiation physics, radiation biology, agriculture, industry, medical, radiation dosimetry, diagnosis, shielding, gamma ray fluorescence, drug delivery, radiation biophysics, science and technology. Mass attenuation coefficient (μ_m), effective atomic number (Z_{eff}), total attenuation cross section, total electronic cross section, effective electron density (N_{eff}), are basic parameter to finding the penetration and energy deposition of gamma radiation [1-9].The theoretical value of the mass attenuation coefficient tabulated of all Elements, mixture and compounds over 1 eV to 100 GeV photon energy ranges [10]. The selected photon energy ranges from 122 keV to 1500 keV are basically used in the medical and biological application during the diagnosis and radiotherapy.The geant4 code freely available http://geant4.fweb.cern.ch/geant4. GEANT4 (GEometry ANd Tracking) simulations used in the field of high energy physics (HEP), atomic nucleus, elementary particles and technology, it gives detail study about radiation interaction with matter. This code applicable for various fields such as radiation physics, radiation biology, medical physics, radio sensitization [11]. The mass energy absorption coefficient and karma of C, N, Si, NaI calculated Steel alloy a comparative study ,composite material a comparative study of Monte Carlo simulation with experimental and theoretical workmeasuring the efficiency of germanium detector using by Geant4 simulation[12-15]. Geant4 Monte Carlo simulation for photon interaction with matter especially electromagnetic physics and interaction process i.e. Photoelectric, Compton, Pair production gives detail study [16].The mass attenuation coefficient of saccharides and amino acids calculated at lower energy, this energy is very useful in medical diagnosis and radiation therapy [17-18]. The atomic number of composite material is depending on the energy, i.e. atomic number of composite material

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decreases with increasing incident photon energy it reflects a number cannot show atomic number of the composite material in entire energy region is called as effective atomic number [19-20].

A variety of physiological functions in the human living system are performed by complex molecule such as amino acid, carbohydrate, protein, fats and oils composed of C, H, N, O element based. Carbohydrates were the most important class of biological material in a living system. It contains sugar, starch, cellulose.

The present study has been shown the validation of Geant4 Monte Carlo simulation compared with experimentally narrow beam geometry and theoretical NIST XCOM database at selected energy region. The study has been undertaken to get information of the mass attenuation coefficient (μ_m), total attenuation cross section, total electronic cross section, molar extinction coefficient, effective atomic number (Z_{eff}), effective electron density (N_{eff}), of the selected carbohydrates with Geant4 monte carlo method. Novelty of present study was to first time applied Geant4 Monte Carlo simulation for measurement of effective atomic number (Z_{eff}) and electron density (N_{eff}) of the C-H-N-O based biological material. We were investigating Geant4 simulation one of the best alternative method for radiation measurement.

Theory:-
Mass Attenuation coefficient:-
The measurement of mass attenuation coefficient of the carbohydrates was performed for homogeneous medium by using Lambert Beer exponential attenuation law,

$$I = I_0 e^{\mu x} \quad (1)$$

Where I_0 and I are the unattenuated and attenuated photon intensity respectively, μ is the linear attenuation coefficient; X is the thickness of the sample. The ratio of linear attenuation coefficients and density of material called as mass attenuation coefficients (μ_m).

Total atomic cross section:-
Firstly, we calculate the total attenuation cross section

$$\sigma_t = \frac{1}{N_A} \sum f_i A_i (\mu_m) \quad (3)$$

N_A is the Avogadro constant, μ_m is the mass attenuation coefficient and A_i is the molar mass of the sample. $\sum f_i = 1$ (f_i is the mole fraction).

Electronic cross section:-

$$\sigma_e = \frac{1}{N_A} \sum_i \frac{f_i A_i}{Z_i} (\mu_m)_i = \frac{\sigma_t}{\sum Z_{eff}} \quad (4)$$

Electronic cross section is the ratio of total attenuation cross section and effective atomic number shows in above written formula.

The effective atomic number (Z_{eff}):-
Compton scattering interaction process of the composite material depends on effective atomic number, which is discussed by [19]

$$Z_{eff} = \frac{\sigma_t}{\sigma_e} \quad (5)$$

Effective Electron Density:-
Effective electron density shows that the number of electron per unit mass

$$N_{eff} = \left(\frac{N_A}{A_{eff}} \right) * Z_{eff} \quad (6)$$

A_{eff} is effective atomic mass also known as the ratio of atomic weight and total number of atom

Experimental detail:-
The radioactive sources [57]Co, [133]Ba, ^{137}Cs, [54]Mn, [22]Na and ^{60}Co were used to generate gamma rays for the experiment. The gamma ray energies emitted by these sources are 122 keV, 360 keV, 511 keV, 662 keV, 840 keV, 1170 keV, 1275 keV and 1330 keV respectively. Gamma rays emitted by these radioactive sources were collimated and detected by the NaI (Tl) scintillation detector. The sources are perpendicular to the surface of the material. The selected gamma ray spectroscopic system was the narrow beam geometry shown in fig 1. As the high Z of iodine in

NaI have good efficiency [21]. The signals from the detector (2"×2") NaI(Tl) crystal having energy resolution of 8.2% at 662 keV gamma rays from the decay of Cs^{137} after suitable amplification according to full width at half maxima FWHM was recorded in EG&G ORTEC 13-bit plug-in-card coupled to a PC/AT. The stability and reproducibility of the arrangement were checked before and after each set of runs in the usual manner. The system shows fine acquires gamma ray spectra to provide accurate information at below room temperature (20 ^{o}C to 23 ^{o}C). All materials had good purity (99 %). The sample thickness was selected in order to satisfy the following ideal condition as far as possible [22].The pellet of material was prepared by using KBr press machine (up to pressure 10 ton) with 0.20 g/cm^2 of uniform thicknesses and confined in a cylindrical plastic container having the same diameter as that of sample pellets. The diameters of the samples were determined with the help of a travelling microscope. Weights of pallet were measured by using digital balance having 0.001 mg accuracy. We measured value of I_o (unattenuated photon intensity) with empty plastic container and I (attenuated photon intensity) with sample at narrow beam geometry set up. The mass attenuation coefficient (μ_m)for all carbohydrate group material was calculated using eq. (1) and theoretically observed by NIST XCOM database at selected incident photon energy. Proper adjustment of the distance between the detector and source (30 cm $\leq$ d $\leq$ 50 cm), the maximum angle of scattering was below 30 min. In the multichannel analyzer used in the present study, there was a built-in provision for dead time correction.

Geant4 Simulation:-
Geant4 Monte Carlo simulation method based on object oriented C++ programming language, it is used for measurement of radiation interaction with matter at wide energy range 250 eV to 100 TeV. Geant4 method for electromagnetic package was especially applied for narrow beam geometry. We were calculated mass attenuation coefficient using computer environment and Geant4 applications G4RunManager for low energy physics Electromagnetic Standard G4PhotoElectricEffect, G4ComptonScattering, G4GammaConversion (pair production). We have known the primary information of electromagnetic package for Geant4 simulation. First stage construction, narrow beam geometry set up and set distance between source-sample-detector. Second stage set energy, chemical composition, density, elemental weight fraction and thicknesses of material, set physical process corresponding to photon energy. Third stage measured simulation value by using GMcalculator after 10^6 times hits of gamma radiation on selected material at particular thickness.

Table 1:- The mean atomic numbers calculated from the chemical formula for the investigated carbohydrates.

	carbohydrates	Chemical Formula	Mean Atomic Number	Molar Mass(g/mol)	A_{eff}
1	Fructose	$C_6H_{12}O_6$	4.00	180.16	7.5067
2	Maltose	$C_{12}H_{22}O_{11}$	4.04	342.30	7.6067
3	Cellulose	$C_6H_{10}O_5$	4.10	342.30	16.2998
4	Sorbitol	$C_6H_{14}O_6$	3.77	182.17	7.0065
5	Raffinose	$C_{18}H_{32}O_{16}$	4.06	504.42	7.6427
6	Xylose	$C_5H_{10}O_5$	4.00	150.13	7.5065

Table 2:- Mass attenuation coefficient (cm^2/g) for the investigated carbohydrates.

Energy (keV)		122	356	511	662	1170	1275	1330
Fructose	Geant4	0.1496	0.1062	0.0923	0.0827	0.0631	0.0603	0.0590
	xcom	0.1546	0.1059	0.0926	0.0839	0.0661	0.0599	0.0595
	NaI(Tl)	0.1424	0.1048	0.0892	0.0815	0.0646	0.0603	0.0570
Maltose	Geant4	0.1492	0.1060	0.0921	0.0826	0.0629	0.0602	0.0589
	xcom	0.1542	0.1056	0.0924	0.0837	0.0659	0.0598	0.0593
	NaI(Tl)	0.1428	0.1028	0.0902	0.0824	0.0634	0.0597	0.0569
Cellulose	Geant4	0.1489	0.1057	0.0919	0.0824	0.0628	0.0600	0.0587
	xcom	0.1538	0.1054	0.0922	0.0835	0.0658	0.0596	0.0592
	NaI(Tl)	0.1404	0.1035	0.0907	0.0811	0.0643	0.0595	0.0572
Sorbitol	Geant4	0.1510	0.1072	0.0932	0.0835	0.0637	0.0609	0.0596
	xcom	0.1560	0.1069	0.0935	0.0847	0.0667	0.0605	0.0600
	NaI(Tl)	0.1468	0.1048	0.0912	0.0835	0.0652	0.0583	0.0585
Raffinose	Geant4	0.1491	0.1059	0.0921	0.0825	0.0629	0.0601	0.0588
	xcom	0.1541	0.1056	0.0923	0.0836	0.0659	0.0597	0.0593
	NaI(Tl)	0.1372	0.0981	0.0904	0.0801	0.0604	0.0578	0.0569
Xylose	Geant4	0.1496	0.1062	0.0923	0.0827	0.0631	0.0603	0.0590

xcom	0.1546	0.1059	0.0926	0.0839	0.0661	0.0599	0.0595
NaI(Tl)	0.1420	0.1031	0.0893	0.0818	0.0647	0.0569	0.0565

Table 3:- Effective atomic number, Z_{eff} of the investigated carbohydrates.

Energy (keV)		122	356	511	662	1170	1275	1330
Fructose	Geant4	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000
	NaI(Tl)	4.0224	4.0097	4.0055	4.0024	3.9957	3.9947	3.9942
	%Error	-0.5569	-0.2419	-0.1373	-0.0600	0.1076	0.1327	0.1452
Maltose	Geant4	4.0444	4.0444	4.0444	4.0444	4.0444	4.0444	4.0444
	NaI(Tl)	4.0815	4.0660	4.0607	4.0570	4.0487	4.0475	4.0469
	%Error	-0.9090	-0.5312	-0.4014	-0.3106	-0.1062	-0.0766	-0.0618
Cellulose	Geant4	4.0952	4.0952	4.0952	4.0952	4.0952	4.0952	4.0952
	NaI(Tl)	4.0815	4.0660	4.0607	4.0570	4.0487	4.0475	4.0469
	%Error	0.3357	0.7182	0.8496	0.9416	1.1485	1.1785	1.1935
Sorbitol	Geant4	3.7692	3.7692	3.7692	3.7692	3.7692	3.7692	3.7692
	NaI(Tl)	3.7279	3.7291	3.7295	3.7298	3.7305	3.7306	3.7306
	%Error	1.1079	1.0753	1.0645	1.0564	1.0374	1.0347	1.0347
Raffinose	Geant4	4.0606	4.0606	4.0606	4.0606	4.0606	4.0606	4.0606
	NaI(Tl)	4.1029	4.0863	4.0807	4.0767	4.0679	4.0665	4.0659
	%Error	-1.0310	-0.6289	-0.4926	-0.3949	-0.1795	-0.1451	-0.1304
Xylose	Geant4	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000	4.0000
	NaI(Tl)	4.0223	4.0096	4.0054	4.0023	3.9956	3.9946	3.9941
	%Error	-0.5544	-0.2394	-0.1348	-0.0575	0.1101	0.1352	0.1477

Table 4:- Effective electron densities, N_{eff} (10^{23} electrons/g) for the investigated carbohydrates.

| Energy (keV)		122	356	511	662	1170	1275	1330
	Geant4	3.1859	3.1759	3.1725	3.1701	3.1648	3.1640	3.1636
Fructose	NaI(Tl)	3.2104	3.2104	3.2104	3.2104	3.2104	3.2104	3.2104
	%Error	-0.7631	-1.0746	-1.1805	-1.2553	-1.4204	-1.4453	-1.4578
	Geant4	3.2328	3.2204	3.2163	3.2133	3.2068	3.2058	3.2053
Maltose	NaI(Tl)	3.2034	3.2034	3.2034	3.2034	3.2034	3.2034	3.2034
	%Error	0.9178	0.5307	0.4027	0.3090	0.1061	0.0749	0.0593
	Geant4	2.9854	2.9854	2.9854	2.9854	2.9854	2.9854	2.9854
Cellulose	NaI(Tl)	3.2436	3.2436	3.2436	3.2436	3.2436	3.2436	3.2436
	%Error	-7.9603	-7.9603	-7.9603	-7.9603	-7.9603	-7.9603	-7.9603
	Geant4	3.2056	3.2066	3.2070	3.2072	3.2078	3.2079	3.2079
Sorbitol	NaI(Tl)	3.2411	3.2411	3.2411	3.2411	3.2411	3.2411	3.2411
	%Error	-1.0953	-1.0645	-1.0521	-1.0459	-1.0274	-1.0243	-1.0243
	Geant4	3.2010	3.2010	3.2010	3.2010	3.2010	3.2010	3.2010
Raffinose	NaI(Tl)	3.2343	3.2212	3.2168	3.2137	3.2067	3.2057	3.2052
	%Error	-1.0296	-0.6271	-0.4912	-0.3952	-0.1778	-0.1466	-0.1310
	Geant4	3.2105	3.2105	3.2105	3.2105	3.2105	3.2105	3.2105
Xylose	NaI(Tl)	3.2284	3.2182	3.2148	3.2123	3.2070	3.2061	3.2057
	%Error	-0.5545	-0.2393	-0.1338	-0.0560	0.1091	0.1372	0.1497
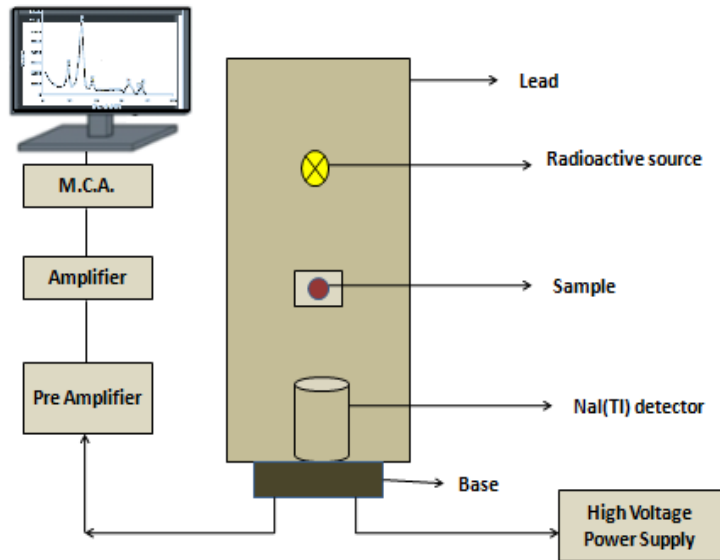
Figure 1:- The schematic view of narrow beam geometry of NaI(Tl) Detector.
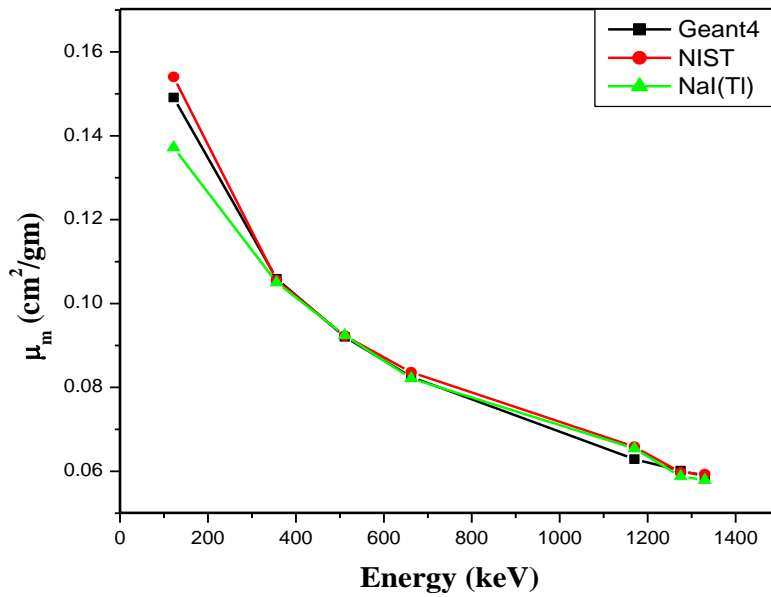

Figure 2:-The typical plot of μ_m versus Energy (E) for Raffinose ($C_{18}H_{32}O_{16}$).
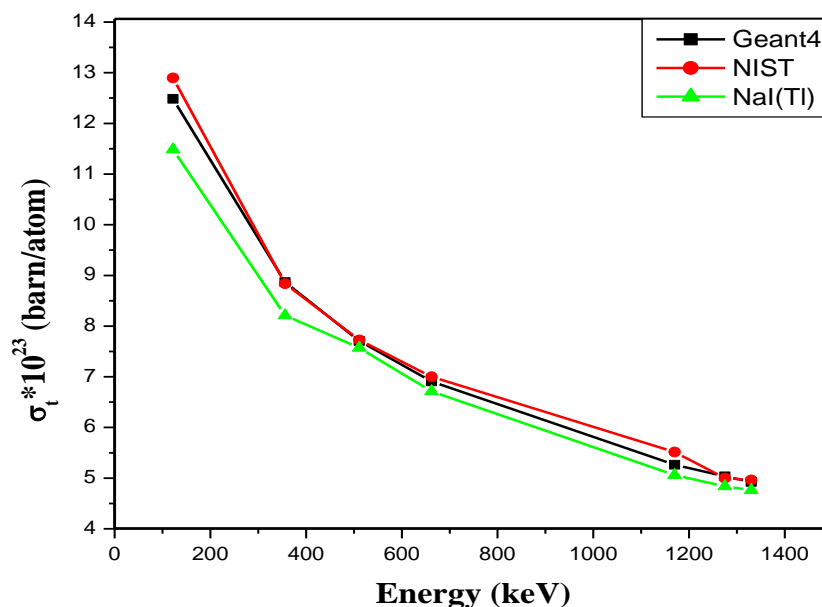
Figure 3:- The typical plot of σ_t versus Energy (E) for Raffinose ($C_{18}H_{32}O_{16}$).
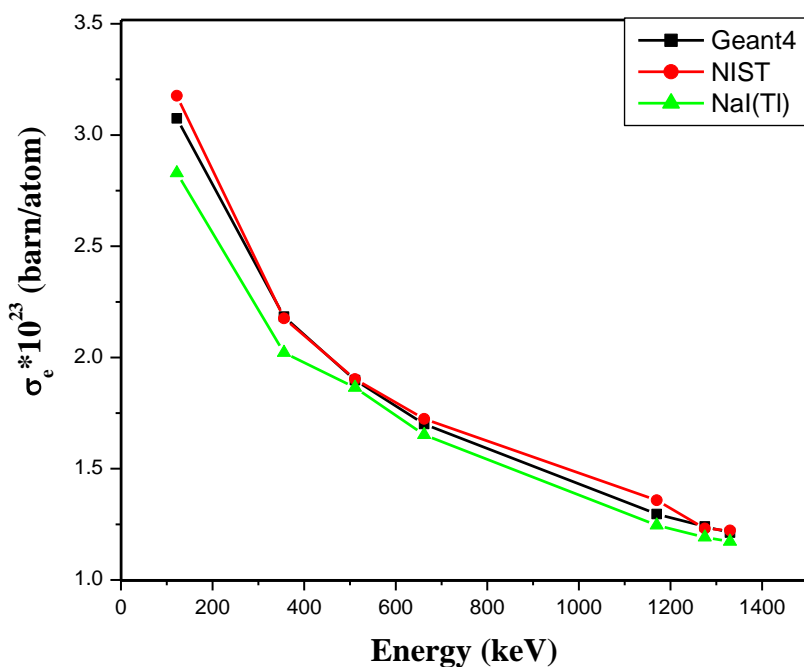

Figure 4:- The typical plot of σ_e versus Energy (E) for Raffinose ($C_{18}H_{32}O_{16}$).

Result and Discussion:-

Comparative NIST XCOM, Geant4 simulation theoretically and experimentally using NaI(Tl) narrow beam geometry study of gamma photon interaction with selected carbohydrates Fructose ($C_6H_{12}O_6$), Maltose ($C_{12}H_{22}O_{11}$), Cellulose ($C_6H_{10}O_5$), Sorbitol ($C_6H_{14}O_6$), Raffinose ($C_{18}H_{32}O_{16}$), Xylose ($C_5H_{10}O_5$) at 122 keV -1330 keV incident photon energy. The table 1 shows the chemical and physical parameter of the sample such as mean atomic number <Z>, molar mass and effective atomic mass calculated by using standard formulae. We studied photon interaction parameter such as the mass attenuation coefficient, total atomic cross section, total electronic cross section, effective atomic number and effective electron density of selected carbohydrate material. The mass attenuation coefficient measured by using Geant4 Monte Carlo simulation this result compared with the NIST XCOM data base and result obtaining from experimental data was determined at 122, 356, 511, 662, 1170, 1170, 1275, 1330 keV photons using

the gamma transmission method by NaI(Tl) narrow beam geometry source-sample-detector set up shown in figure 1. In the selected energy Compton scattering is main interaction process, i.e. Compton scattering is dominance in this selected energy region and photoelectric effect is prominent.

The mass attenuation coefficient of carbohydrates study tabulated in table 2 and graphically represent in figure 2. We observe the mass attenuation coefficient measured from NIST XCOM, Geant4 Monte Carlo simulation and experimentally by NaI(Tl) narrow beam geometry values with respect to incident photon energy were nearly equal to each other. The mass attenuation coefficient was sharply decreased with increasing incident photon energy. It shows the mass attenuation coefficient is depending on the incident photon energy and chemical composition of the material. The μ_m is most important basic physical quantity for radiotherapy, medical physics, radio sensitization and computations of radiation measurement quantities.

The theoretical information about total attenuation cross section and electronic cross section by using the mass attenuation coefficient (Geant4, XCOM and NaI(Tl) scintillation detector) calculates from equation 3 and 4. Graphically in figure 3 and 4 shows the value of the total attenuation cross section and electronic cross section was linearly decreased with photon energy increased of the carbohydrate. The parameter total and electronic cross sections having main purpose to measuring the distribution of photon flux in the object. The table 3 and table 4 gives information about effective atomic number and effective electron density of the material. It shows no change in Z_{eff} and N_{eff} in the selected energy region. It indicate no change in Z_{eff} calculated by using Geant4/NaI(Tl) scintillation detector, it reflects that Compton scattering was main interaction process their multiple scattering occur that's why photon living longer time in material. Our result compares with other literature gives same information photon energy increases the Z_{eff} was decreased, but their Compton scattering was main interaction process their Z_{eff} remain constant. The Z_{eff} calculated by using NaI(Tl) detector results compared with Geant4 monte carlo simulation method results it gives same information on the selected energy region. The Z_{eff} and N_{eff}error found between Geant4 simulation and NaI(Tl) scintillation detector at 122- 1330 keV for all carbohydrates shown in table 3 and 4. We measured error in between Geant4 and NaI(Tl) by using eq

$$\% \text{ Error} = \frac{Z_{eff}[\text{Geant4}] - Z_{eff}[\text{NaI(Tl)}]}{Z_{eff}[\text{NaI(Tl)}]} * 100$$

We observed that the Geant4 simulation method was valid for measuring Z_{eff} of C-H-N-O based material. We observed the highest electron density of the Raffinose was $3.23*10^{23}$ at 122 keV, it depends on the increasing total and electronic cross section this study reflects the classification of tumor i.e. effected tumor having a higher electron density than other tissue [23]. The use of Z_{eff} for the medical and biological application and the N_{eff} which used for measuring distribution of photon or deposition of photon in biological, shielding and dosimetric material [24].

Conclusion:-
We performed experiment using NaI(Tl) narrow beam geometry set up at 122 keV, 360 keV, 511 keV, 662 keV, 840 keV, 1170 keV, 1275 keV and 1330 keV photon energy from carbohydrates. We have done work with Geant4 Monte Carlo simulation at selected energy region. Experimental measured mass attenuation coefficient (μ_m), total attenuation cross section (σ_t), electronic cross section (σ_e) comparing with Geant4 Monte Carlo simulation and NIST standard data base having good agreement with each other. The important part of this study is experimentally measured and simulated value of the effective atomic number and the effective electron density cannot shows the variation in a given energy region. We calculate effective atomic number from eq. 6 was also agreed with available data having less error. We conclude that Geant4 is a useful simulation toolkit in medical radiation, biophysics and theoretically Z_{eff}will be calculated for C-H-N-O based materials.

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Conflict of Interest:-Author has no conflict of interest

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