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Monte Carlo simulation for the estimation of iron in human whole blood and comparison with experimental data

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Abstract. Monte Carlo N-particle (MCNP) code has been used to simulate the transport of gamma photon rays of different energies (22, 31, 59.5 and 81 keV) to estimate the iron content in solutions. In this study, MCNP simulation results are compared with experiment and XCOM theoretical data. The simulation shows that the obtained results are in good agreement with experimental data, and better than the theoretical XCOM values. The study indicates that MCNP simulation is an excellent tool to estimate the iron concentration in the blood samples. The MCNP code can also be utilized to estimate other trace elements in the blood samples.

Keywords. Attenuation coefficient; Monte Carlo N-particle-4C code; blood.

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1. Introduction

Study on interaction of photon with compounds or mixtures has become an important research area for shielding and dosimetry. Data on the attenuation of X-/γ-ray photon with matter are required for medical application, industries, agriculture, nuclear power plants, etc. Photon energy and chemical compositions are required to investigate photon interaction parameters with different types of elements, materials and compounds (e.g. human body organs, tissues, dosimetric materials, shielding materials, etc.). Recently, mass attenuation coefficients have been utilized to estimate heavy metal elements in different matrices [1].

Trace elements ($<0.1\%$) are essential for biochemical conversions inside the body. Neutron activation analysis, total reflection X-ray florescence and computed induced by neutron are some useful techniques for the estimation of trace elements [2–6]. One of the most vital constituent in the human body is blood which contains H, C, N, O elements (99%) and Na, P, S, Cl, K and Fe elements (1%) [7]. Blood samples are being tested for disease, mineral content, organ function etc. The routine testing of blood samples requires a robust and easy method.

Measurement of iron in human whole blood is a routine and reliable means for assaying the amount of hemoglobin (Hb) in blood. World Health Organization has defined normal Hb level for an adult man, pregnant and non-pregnant adult women and the minimum Hb level for human whole blood for both men and women. The greater increase in blood volume compared to red blood cells will result in lower Hb levels and this condition is called the physiological anemia of pregnancy.

The routine blood sample analysis for pregnant women requires a large number of samples. Presently, various methods are available (where samples cannot be recovered after analysis) in hospital for large-scale blood test which require standard procedural adherence, and are time-consuming. The techniques should be reliable, cheap, simple, and easy to use [8,9]. Recently, a new experimental technique called photon attenuation technique has been reported for the detection of Hb in blood [10].

Modelling of photon transport through human whole blood in a computer environment provides greater flexibility for multiple experimental measurements for different photon energies without radiological safety concern. An elemental analysis on gold, bronze and water matrix has been reported recently using MCNP [1]. Similarly, it is possible to estimate the iron content in blood using MCNP. The main objectives of the present study are to test the validity of MCNP simulations to demonstrate its success in studying radiation interactions in blood samples to estimate iron concentration (Hb level) and also to investigate other trace elements in blood samples.

2. Computational methods

2.1 *Monte Carlo simulations*

MCNP is a general-purpose Monte Carlo code for transport of neutrons, photons and electrons. MCNP is a continuous-energy, generalized geometry, time-dependent, coupled neutron–photon–electron Monte Carlo transport code system. The program is based on Monte Carlo N Particle transport (MCNP-4C) code developed by Los Alamos National Laboratory. The MCNP-4C uses physics models for particle interactions and nuclear cross-section libraries. The user can apply up to second-order surfaces (boxes, ellipsoids, cones, etc.) and fourth-order torii to build a 3D geometry which can be filled with materials of arbitrary composition and density. Point, surface or volume sources of radiation can be defined, from which the mentioned particles are emitted with user specified probability distributions for energy and direction. The code then simulates the particle tracks and interactions in the materials, according to probability density distribution [11].

The simulated geometry consisted of a cubic model of $10 \times 10 \times 1$ cm^3 dimension. The environment was filled with air. Finally, the cubic model was centred in an air sphere for variance reduction. Anything outside the air cube was considered void into which MCNP did not allow particle transport. Tally F2 was used to obtain MCNP-4C simulation data. This tally calculates flux in the cube sides for every source. The MCNP source was modelled as a directional plane source in vacuum. This source was located 10 cm away from the entry plane of the mentioned cube. The initial direction of gamma source was parallel to the beam axis. Simulations were performed with 100000 histories. All simulation data obtained by MCNP code are found with less than 2% error.

2.2 *XCOM program*

The mass attenuation coefficient, μ/ρ, for compounds or composites are calculated by using mixture rule

$$(\mu/\rho)_{\text{blood}} = \sum_{i}^{n} w_i (\mu/\rho)_i ,$$

where w_i is the proportion by weight and $(\mu/\rho)_i$ is the mass attenuation coefficient of the ith element by using XCOM [12]. The $(\mu/\rho)_{\text{blood}}$ values were used for the detection of Hb level in the human whole blood samples.

The uncertainties in μ/ρ values are about 1% for low-Z ($1<Z<8$) in Compton region (30 keV to 100 MeV). Below 30 keV energy, the uncertainties are 5–10% because of correction to experiments for high-Z impurities and departure of Compton cross-section from Klein–Nishina theory. Also, above 100 MeV photon energy, uncertainties may be 5–10%. The gamma sources of photon energies above 5 keV are being used in medical, biological, industrial, radioactive source transportation and other shielding applications. Hence, uncertainty in our results may not have any impact for practical applications.

3. Results and discussion

The computation work on the estimation of iron concentration in human whole blood samples was done in five steps: (i) mass attenuation coefficients for iron solutions, (ii) iron content in water, (iii) mass attenuation coefficients for iron containing blood solutions, (iv) iron in blood solution and finally (v) Hb in patient blood samples. The MCNP simulation results were compared with theoretical XCOM and experimental data at 22, 31, 59.5 and 81 keV photon energies.

3.1 *Simulation*

First of all, the MCNP simulation was carried out for an iron solution containing 5, 2.5, 1.25 and 0.625 g/ml iron. The MCNP simulation results, XCOM values and experimental data for mass attenuation coefficients for 22, 31, 59.5 and 81 keV photon energies are given in table 1 and a good agreement is observed. Known amount of iron was added in water and then the solution was analysed for the estimation of iron using MCNP, XCOM and experiment at 22, 31, 59.5 and 81 keV photon energies. The results for water are given in table 2, showing a very good agreement for MCNP with XCOM and experimental data.

Table 1. Comparison of experimental and theoretical mass attenuation coefficients (in cm^2/g) for iron solution at low photon energies.

	Mass attenuation coefficients (cm^2/g)											
	22 keV			31 keV			59.5 keV			81.0 keV		
Added (g/ml)	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.
5	0.838	0.950	0.945	0.400	0.468	0.452	0.199	0.222	0.217	0.175	0.188	0.171
2.5	0.693	0.800	0.720	0.348	0.413	0.405	0.192	0.214	0.209	0.172	0.185	0.169
1.25	0.619	0.729	0.718	0.320	0.385	0.382	0.189	0.210	0.189	0.171	0.184	0.165
0.625	0.587	0.610	0.622	0.309	0.372	0.370	0.188	0.208	0.188	0.171	0.183	0.155

Table 2. The experimental and calculated values of the detected iron in water.

	Iron content in water (g/ml)											
	22 keV			31 keV			59.5 keV			81.0 keV		
Added (g/ml)	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.
5	5.00	4.90	4.88	4.89	4.33	4.27	4.89	4.80	3.36	4.70	4.58	ND
2.5	2.50	2.48	2.17	2.46	2.45	2.13	2.39	2.38	0.75	1.93	1.13	ND
1.25	1.25	1.23	1.18	1.19	1.20	1.08	1.18	1.08	ND	0.90	0.59	ND
0.625	0.62	0.62	0.61	0.60	0.60	0.52	0.52	0.42	ND	0.055	0.053	ND

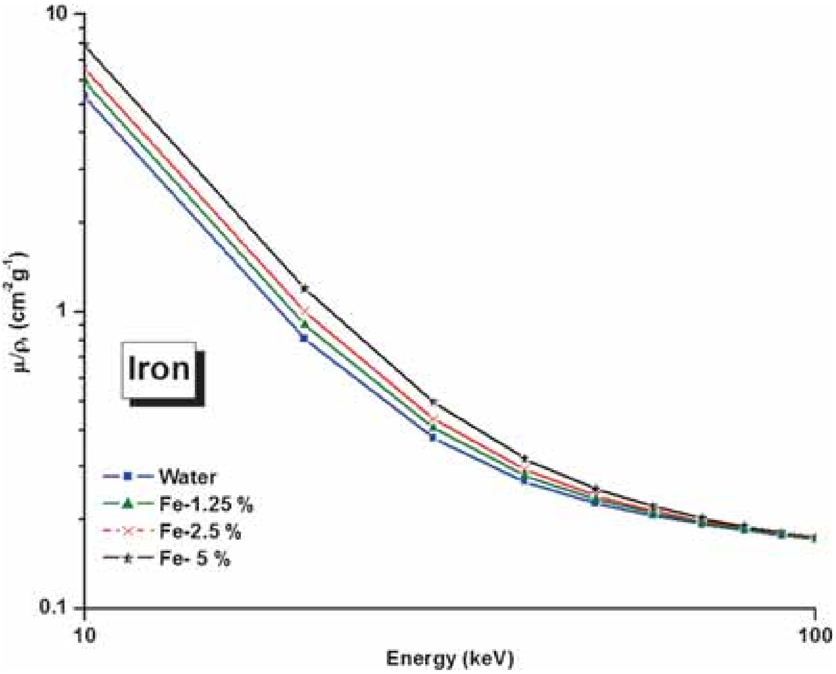

Figure 1. The generated MCNP mass attenuation coefficients of iron solution with different concentrations at low energy range (10–100 keV).

The MCNP mass attenuation coefficients calculated for water after adding 5, 2.5 and 1.25% of iron impurities in low energy range (10–100 keV) are shown in figure 1. The curves indicating low concentration of impurity are at the lower side of the figure while curves indicating high concentration is at the upper side. It is to be noted that the iron content in water was found close to the added amount by MCNP, XCOM and experiment for 22 keV and difference increase with the energy. At 81 keV energy, the iron content could not be detected in the experiment.

The mass attenuation coefficients for blood solutions at 22, 31, 59.5 and 81 keV photon energies for different iron contents are given in table 3. The simulated

Table 3. Comparison of experimental and theoretical mass attenuation coefficients (in cm^2/g) for blood solution at low photon energies.

	Mass attenuation coefficients (cm^2/g)											
	22 keV			31 keV			59.5 keV			81.0 keV		
Added (g/ml)	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.
5	0.857	0.972	0.945	0.405	0.428	0.415	0.200	0.222	0.210	0.174	0.189	0.180
2.5	0.713	0.825	0.720	0.354	0.421	0.399	0.193	0.214	0.198	0.172	0.186	0.179
1.25	0.692	0.751	0.718	0.347	0.393	0.360	0.192	0.210	0.197	0.172	0.184	0.178
0.625	0.699	0.610	0..622	0.349	0.367	0.355	0.192	0.207	0.195	0.172	0.183	0.177

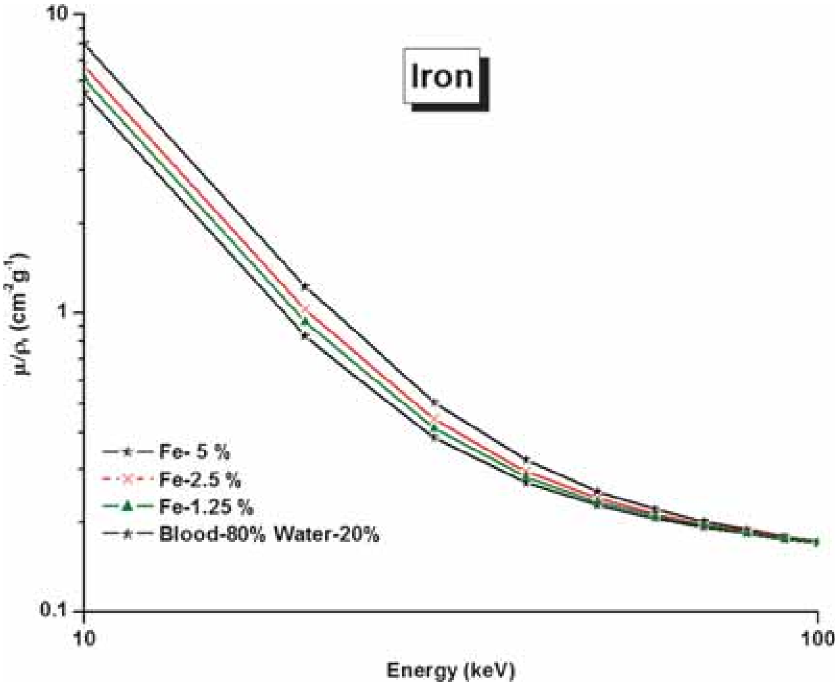

Figure 2. The generated MCNP mass attenuation coefficients of blood solution with different iron concentrations at low energy range (10–100 keV).

Table 4. The experimental and calculated values of the detected iron in blood solution.

	Iron content in blood solution (g/ml)											
	22 keV			31 keV			59.5 keV			81.0 keV		
Added (g/ml)	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.	MCNP	XCOM	Exp.
5	5.00	4.90	4.88	5.00	5.04	4.91	4.88	4.67	4.36	4.50	4.48	ND
2.5	2.50	2.48	2.17	2.49	2.53	2.49	2.39	2.36	1.751	1.69	1.67	ND
1.25	1.25	1.23	1.18	1.22	1.23	1.19	1.15	1.12	N.D	1.17	1.12	ND
0.625	0.62	0.62	0.61	0.60	0.60	0.6	0.61	0.61	N.D	0.58	0.50	ND

MCNP mass attenuation coefficients for blood solution after adding 5, 2.5 and 1.25% of iron impurities in low energy range are shown in figure 2.

A very good agreement of MCNP with XCOM and experimental data was observed for mass attenuation coefficients for blood solutions (see table 3). The iron content in the blood samples was estimated by MCNP, XCOM and experiment for the same energies (22, 31, 59.5 and 81 keV), and a good agreement was noted between theoretical and experimental values (see table 4).

3.2 *Comparison with experiment*

The mentioned simulation method was applied for different human whole blood samples [9] containing

Table 5. Comparison of experiment [10] and theoretical estimation of hemoglobin in some patients.

	Patient history				Hemoglobin (g/dl)		
Blood sample	Gender (M/F)	Age	Weight (kg)	Hemoglobin (g/dl)	MCNP	XCOM	Exp.
1	M	5	17	8.70	8.65	8.90	8.50
2	M	7	24	10.12	10.18	11.00	10.56
3	M	12	30	11.35	11.82	11.87	10.82
4	F	4	16	8.90	8.86	9.12	8.89
5	F	13	34	11.11	11.46	11.78	11.36
6	F	16	47	12.10	12.14	13.00	12.35
7	M	25	60	11.40	11.33	12.13	11.23
8	M	30	67	13.15	13.16	14.12	13.56
9	M	36	73	14.15	14.12	14.24	14.02
10	F	23	56	11.23	11.60	11.80	11.60
11	F	29	63	12.13	11.18	12.08	11.88
12	F	35	71	13.18	13.32	13.90	13.50
13	M	40	72	14.25	14.11	14.76	14.33
14	M	45	69	13.89	14.00	14.25	14.01
15	F	45	71	12.14	12.24	12.89	12.34
16	F	47	75	13.10	13.10	13.68	13.44
17	F	50	65	14.15	14.10	14.98	14.19
18	M	55	69	13.75	13.65	14.25	13.95
19	M	50	82	14.30	14.40	14.93	14.45
20	M	57	89	14.25	14.13	14.84	14.43

different Hb levels. The human whole blood samples were taken from child, adult and old patients with Hb ranging from 8 to 15 g/dl. The Hb was detected using MCNP simulation, XCOM and experiment. Table 5 compares the present simulation results, theoretical XCOM and experimental data for Hb concentration. A very good agreement was seen among the MCNP, XCOM and experimental data.

4. Conclusion

In this study, the mass attenuation coefficients and iron content for human whole blood samples were estimated using MCNP simulation and results were compared with experimental data and the XCOM code. The simulation shows that the obtained results are very close to experimental data and better than the theoretical values. The results indicate that MCNP simulation is a very good tool to estimate the iron concentration in blood samples.

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