Study the Variation of Gamma - Ray Backscattered Count Rate for Halley's Nucleus

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Abstract

In this paper, the single scatter model for gamma backscatter densitometer has been used to investigate the materials of Halley's nucleus. Monte Carlo simulation tool is used for the evaluation and calibration of gamma backscatter densitometer; and also used to calculate the bulk density. A set of parameters effecting detected count rate of γ – ray backscattering, mainly the source energy, the source – detector separation (sonde length), density and composition, were calculated.
Results obtained with the present method are compared with experimental data and the computed data may be considered entirely satisfactory.

Keywords: Comet, density, Compton backscatter, Monte Carlo, single scatter model.

دراسة التغير في العد للأستطارة الخلفية لأشعة كاما لنواة المذنب هالي

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الخلاصة:

في هذا البحث، استعملت الأستطارة المنفردة لأشعة كاما المرتدة او المنعكسة في مقياس الكثافة الظاهرية للبحث عن تركيب المواد في نواة المذنب هالي. كما استعملت محاكاة مونتي كارلو كأداة لتقييم و تدريج مقياس الكثافة لاشعة كاما المرتدة، التي ساهمت ايضاً في حساب الكثافة الظاهرية. لقد تم حساب مجموعة المعلمات المؤثرة في معدلات العد لاشعة كاما المنعكسة مع مصدر طاقة اشعة كاما، المسافة ما بين المصدر المشع والكاشف، الكثافة وايضاً تركيب عناصر نواة المذنب.
لقد قورنت النتائج المستحصلة للتقنية الجديدة المستعملة مع البيانات العملية والمحسوبة وكانت متوافقة بشكل جيد.

Introduction:

Gamma backscatter density densitometer uses the Compton scattering of γ ray photons in bulk material to measure density near the surface of comet nucleus [1]. This technique is widely used in physics, industry and astronomy. Gamma backscatter density densitometer has even been adapted for use on measurement were built and launched to the Moon, Mars and Venus for a review of lunar surface bulk density data. Bulk density measurement has also been suggested for the BepiColombo Mercury lander, as part of

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a heat flow and physical properties package. The Rosetta mission to comet Wirtanen is one of the missions that allow to physical properties of cometary nucleus material to be measured in situ for the first time [2, 3]. This technique depends on the detection and analysis of scattered photons at the surface of a bulk material which is being irradiated by a source placed some distance away [1].

The single scattering model (SSM) has been used to explain the basic behaviour of backscatter densitometers. Monte Carlo methods are preferred for modelling real devices but the SSM is used for examining basic features of the measurement technique.

Comets are solid bodies with a high volatile content, the vaporization of which makes them obvious when they approach the Sun [4].

Comets consist of three parts: Nucleus which is the only part of a comet present at all times, Coma and Tails.

The most important part that will be studied in this research is comet nucleus because it is thought to contain primordial material which has remained relatively unchanged since the formation of the solar system. Any modification of this material is most likely to be evident at the surface of the nucleus [5].

The SSM assumes that photons reaching the detector have been scattered only once in the material [1].

Cometary nuclei are now established to be solid bodies comprising a mixture of ices (Dominated by H_2O and CO), minerals (e.g. silicates of Fe, Mg, Ca and Al) and Hydrocarbon compounds (containing C, H, O, N) [6].

The most famous comet, associated with many important events in history that will be studied is Halley [5].

Simulation procedure:

The computer program that calculated backscatter of gamma rays is designated and written for the calculation in the geometrical arrangement of Compton backscattered densitometer as shown in figure 1. A source of gamma photons (usually 662 keV and 60 keV from a collimated ^{137}Cs and ^{241}Am respectively sources) is placed at the surface of the bulk sample to inject gamma photons into the material.

A photon detector D (NaI) with radius (RD) is placed a short distance (d) along the surface from the source to count photons scattered out of the material.

A general path for singly scattered photons is shown in the geometry, the direction of the emitted photon being at an angle α to the baseline SD.

Compton scattering is assumed to occur at a point P in the material, though some proportion of the photons may not reach P, having undergone absorption or scattering somewhere along the path SP of length r_1.

Those photons scattered at P towards the detector make an angle β with baseline and may of course be lost along the path PD (of length r_2).

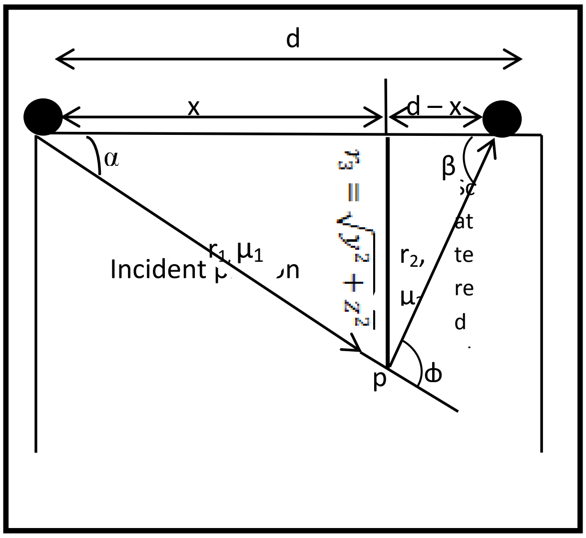


Figure 1- Basic geometry for a Compton backscatter densitometer

The material under investigation is assumed to be of a uniform density ρ. The mass attenuation coefficient μ for photons is a function of their energy. Since one assumes a mono – energetic source (such as the most commonly used radioisotope ^{137}Cs which emits at 662 keV), the attenuation coefficient μ_1 for primary photons was fixed and the mass attenuation coefficient for scattered photons μ_2 varies with the new photon energy after Compton scattering. This is done by random sampling of the Klein – Nishina distribution. The most appropriate sampling method for this application is the Kahn method, which is not an approximation and works for any incident photon energy. The method requires generating and analysis of at least one set of these random numbers (υ_1, υ_2, υ_3) in the range $0 \leq \upsilon_i \leq 1$ [6].

The procedures for a single Compton event is shown in figure 2.

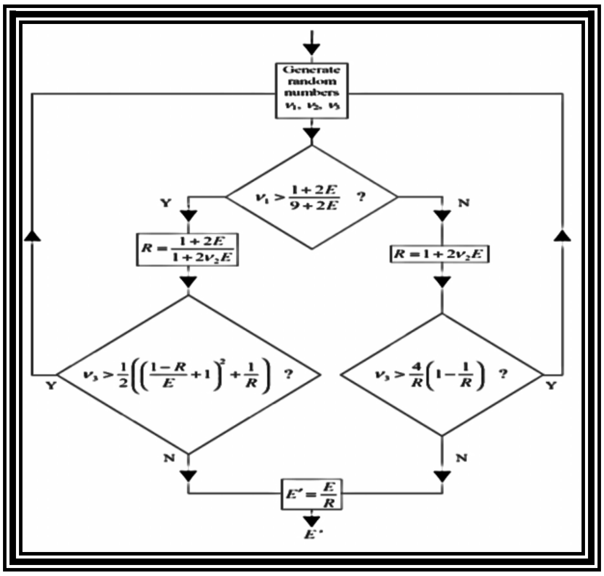


Figure 2- method for random sampling of the Klein – Nishina distribution by Kahn method [6].

Using simple trigonometry one can obtain the basic relations between the angular and linear parameter in the diagram. These are useful when transforming between angular and Cartesian coordinate system and when writing computer program.

$$\mathbf{r_1^2 = x^2 + y^2 + z^2,}$$
$$\mathbf{r_2^2 = (x-d)^2 + y^2 + z^2}$$
$$\mathbf{r_3 = \sqrt{y^2 + z^2}}$$
$$\boldsymbol{\varphi = \alpha + \beta}$$
$$\boldsymbol{\alpha} = \mathbf{tan^{-1}\frac{\sqrt{y^2+z^2}}{x}}, \quad \boldsymbol{\beta} = \mathbf{tan^{-1}\frac{\sqrt{y^2+z^2}}{d-x}}$$

To model the Compton backscatter design, Monte Carlo program has been written to describe the absorption and scattering of photons in bulk material [1, 6].

A flowchart of the Monte Carlo algorithm is given in figure (3) contains all auxiliary operations beginning from the data reading and ending with the printing of the results. It is divided into a main program and twelve subprograms for the data preparation and interpolation.

Tables (1 and 2) containing attenuation coefficient for various elements of Halley with respect to gamma – ray energy were used as the input of the program. The program calculated single scattering of each photon and gains the values of the Compton backscatter simultaneously for various values of twelve elements, detector positions. The program was designed in FORTRAN language (77-90) for personal computer (pc).

Monte Carlo algorithm

The photon source is assumed to be a point source and located at the surface of a semi - infinite bulk material of uniform density. Monte Carlo simulation is used to follow a large number of photon histories in order to determine the distribution of the backscattered radiation.

A random number generator is used to obtain a uniform distribution of random number υ in the range $0 \leq \upsilon < 1$.

Simulation of a single photon history requires the following steps:

- Input data such us dimension, density of the bulk martial, radius of the detector used and number of photons incident.
- Input values of mass attenuation coefficients of materials.
- Sampling for source energy has been used by two monochromatic sources, such as ^{137}Cs and ^{241}Am which for one emission peak each, also we used range of energies.
- For computing the mass attenuation coefficient of incoherent μ at various values of gamma – ray energies for the materials were obtained using the interpolation function.

- A photon is emitted in random direction (θe,φe), having energy EG. cosine – sampling has been used for the polar angle θe and uniform sampling for the azimuthal angle φ:

$$\theta_e = \cos^{-1}(2\upsilon_1 - 1)$$
$$\varphi_e = \pi\upsilon_2$$

Where υ is the random number $(0 \leq \upsilon \leq 1)$.

- The free – flight distance PL traveled by the photon in material is found by using [7]:

$$\mathrm{PL} = -\frac{1}{\mu(E)}\ln(1-R)$$

- The equation of the line defined by the photon path is given by:

$$\vec{r} = \vec{r_\circ} + t\,\vec{n}$$

Where n is the vector along the direction of the photon path and t is a variable parameter and the parametric equations are:

$$x = x_\circ + t\,n_x$$
$$y = y_\circ + t\,n_y$$
$$z = z_\circ + t\,n_z$$

Where (n_x,n_y,n_z) are the compounds of the vector n and (x_o, y_o, z_o) are the coordinates of the emitter point in the source and (x_o, y_o) can be calculated from equations:

$$x_o = \upsilon_3 A - \frac{A}{2}$$

$$y_o = \upsilon_4 B - \frac{B}{2}$$

Where A and B are dimensions of the source [2, 6].

- The new photon energy after Compton scattering was obtained using Khan Method. The method needs to generate and analysis these random numbers (υ_3, υ_4, υ_5) in the range ($0 \leq \upsilon \leq 1$).
- Calculation of the polar of scattering using Compton formula is given by [8]:

$$\cos\theta = 1 - \left(\frac{1}{E'} - \frac{1}{E}\right) m_o c^2$$

Where E and E' are old and new energies and $m_o c^2$= 0.511 MeV.

- Checking the three conditions to complete the calculation processes:

1. $PL_i \leq r_1$.
2. $PL_s \geq r_2$.
3. $45^\circ \leq \alpha < 90^\circ$.

Where PLi is the path length of incident photon and PLs is the path length of scattered photon.

Table 1- Attenuation coefficient with respect to gamma – ray energy (0.001 - 0.05) MeV, density and abundance of Halley's material [9, 10]

Molecule	Density g/cm^3	abundance	Mass attenuation coefficient (μ/ρ) = cm^2/g				
			Energy = MeV				
			0.001	0.002	0.005	0.01	0.02
H_2O	0.917	100	4086.6	618.7	42.72	5.38	0.85
CO	0.789	3.5	3544.5	225.80	35.32	4.38	0.67
CO_2	1.562	3	3109.47	462.189	31.3677	3.89571	0.592956
CH_4	0.442	< 1	1664.71	228.31	14.744	2.1625	0.7005
C_2H_2	0.729	0.3	4080.768898	559.501028	35.3230422	4.434233	0.8726842
C_2H_4	0. 567	0.3	3792.058352	519.947472	32.9767328	4.282092	0.9683608
C_2H_6	0. 546	0.4	3544.652	486.072	31.0628	4.254	1.15
CH_3OH	0. 791	1.7	3144.25343	464.13937	32.30403	4.95859	1.64759
H_2CO	0. 815	< 0.4	3331.43614	491.77704	33.226846	4.17094	0.687291
NH_3	0.817	1.5	2729.59188	393.36918	26.079132	3.39846	0.703755
HCN	0. 697	0.2	2696.08677	381.65722	24.761103	3.076365	0.530025
H_2S	1.540	0.41	2287.46636	362.40796	328.457604	47.18876	6.356914

Table 2- Attenuation coefficient with respect to gamma – ray energy (0.05 - 2) MeV of Halley's material [9, 10]

Molecule	Mass attenuation coefficient (μ/ρ) = cm^2/g					
	Energy = MeV					
	0.05	0.1	0.2	0.5	1.0	2.0
H_2O	0.26	0.20	0.16	0.11	0.08	0.0589
CO	0.19	0.15	0.11	0.08	0.06	0.04407
CO_2	0.167349	0.125853	0.101283	0.0714714	0.052143	0.0364728
CH_4	0.47625	0.40725	0.33525	0.2384	0.1737	0.121
C_2H_2	0.3968788	0.3239632	0.2644314	0.1875786	0.1367844	0.09545066
C_2H_4	0.5124412	0.4267468	0.3496236	0.2482784	0.1809816	0.12619584
C_2H_6	0.7024	0.5944	0.4884	0.34712	0.25296	0.17628
CH_3OH	1.132125	0.970187	0.799156	0.568318	0.4140125	0.288346
H_2CO	0.233353	0.182411	0.147854	0.1045929	0.0762761	0.051705
NH_3	0.340461	0.2812275	0.2295945	0.1631532	0.1189026	0.08295135
HCN	0.198024	0.157176	0.127317	0.0902874	0.0658452	0.0460095
H_2S	0.589461	0.224186	0.150518	0.1026878	0.0745577	0.0525182

Definitions

SL = sonde length (source – detector separation) (cm).

SX= distance between source and R_3 (cm).

XD= distance between R_3 and the detector (cm).

RD= radius of detector (cm).

N_t= number of photons (10^6).

E_G= energy of gamma (keV).

ρ_o = density (g/cm^3).

μ = mass attenuation (cm^2/g).

E_{in}= incident energy (keV).

E_S= scattered energy (keV).

R = random number.

θ_{em} = emitting angle.

φ_{em} = azimuthal angle.

n_x, n_y, n_z = unit vectors.

PL_{in}= path length of incident photon.

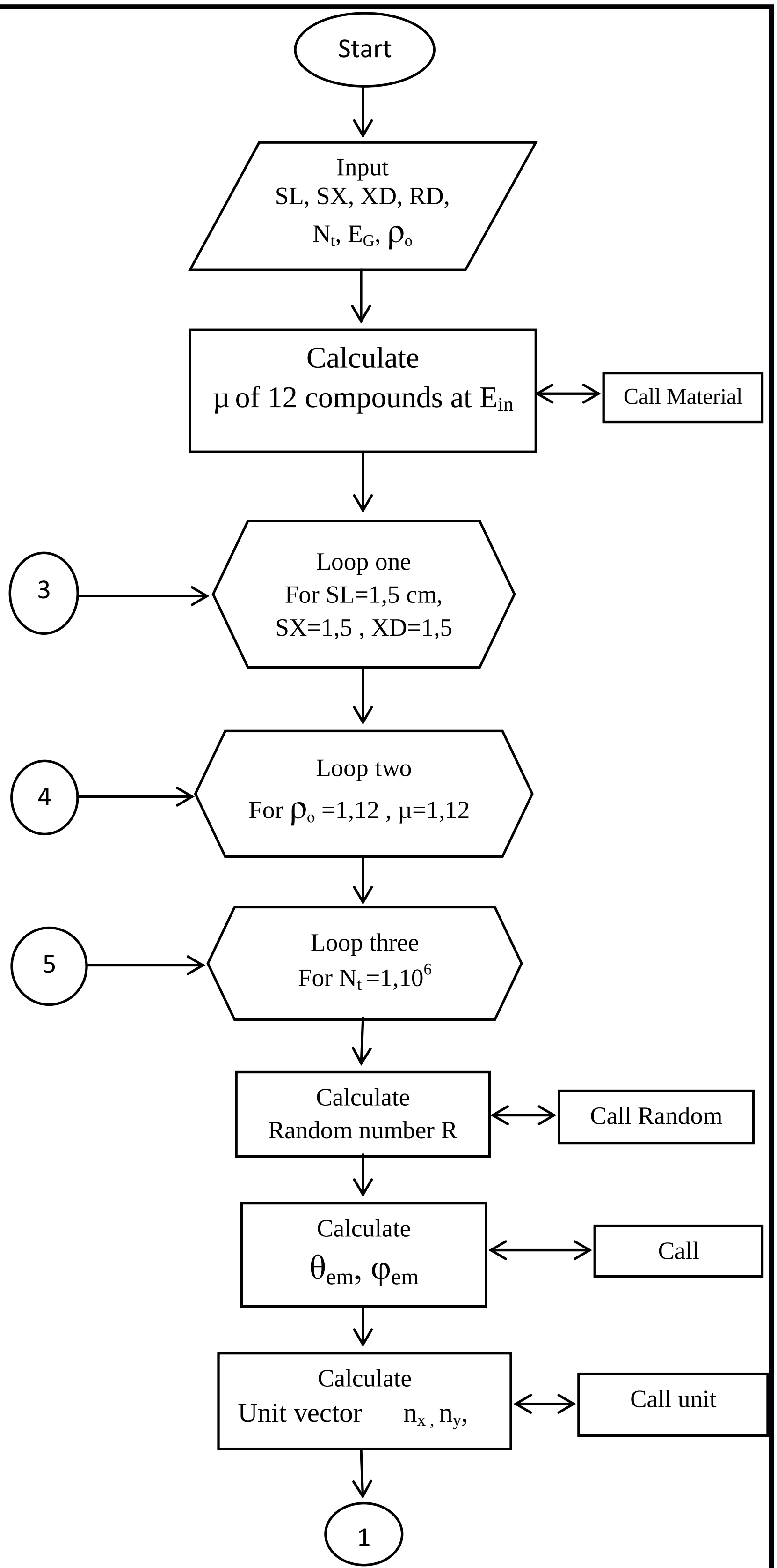
PL_S= path length of scattered photon.

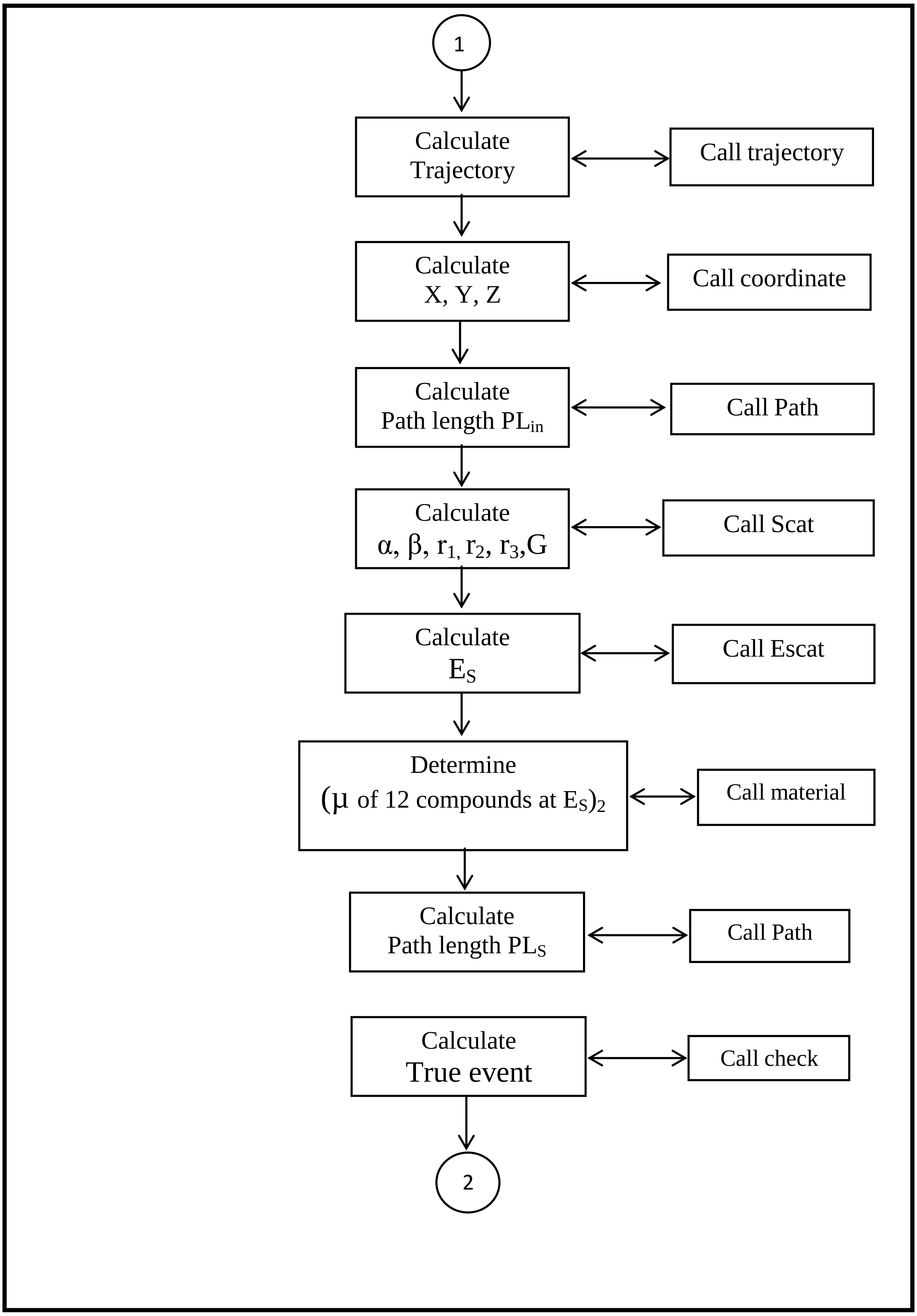
r_1= distance of SP.

r_2= distance of PD.

r_3= $\sqrt{y^2+z^2}$.

X, Y, Z = coordinates.




1
Calculate Trajectory
Call trajectory
Calculate X, Y, Z
Call coordinate
Calculate Path length PL_{in}
Call Path
Calculate α, β, r_1, r_2, r_3, G
Call Scat
Calculate E_S
Call Escat
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Call Path
Calculate True event
Call check
2

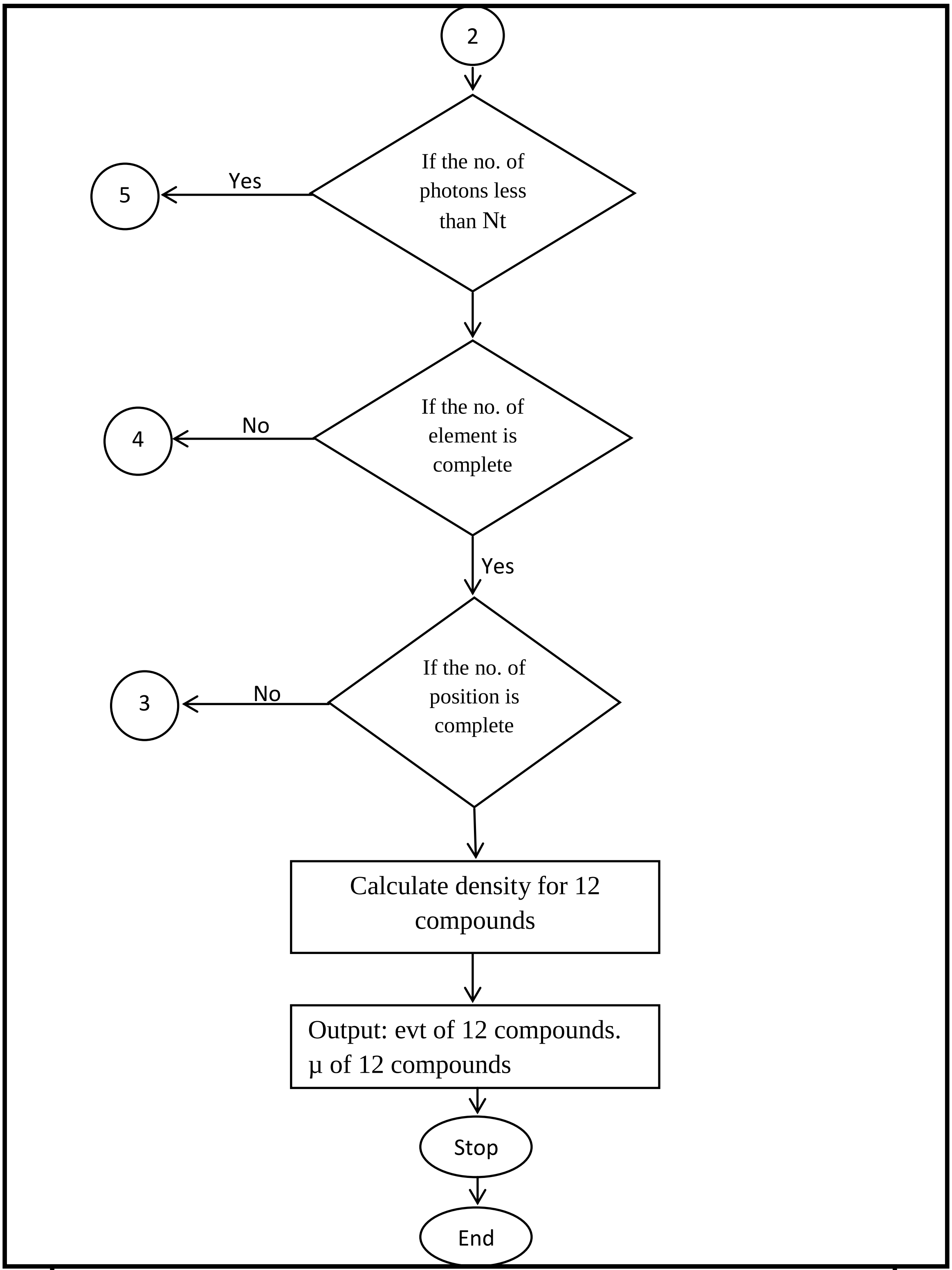


Figure 3- flowchart of the Monte Carlo algorithm

Results and discussions:

In this work, Monte Carlo simulation of Compton backscatter densitometer in semi – infinite bulk materials have been used to:

First: calculate the bulk density by comparing the number of photons entered and detected; also the count rate should be independent of composition.

If the number of counts detected in a sonde length (1,2,3,4, and 5) cm is N_o with no intervening material but N once a material has been introduced, the bulk density ρ_{bulk} is given by

$$\rho_{bulk} = -\frac{1}{\mu z}\ln\frac{N}{N_o}$$

Where μ is the mass attenuation coefficient at 662 keV, z is the path length of photon from the source to the detector through the material.

By comparing the results of five sonde lengths with real density for two comets materials chose the closest result for those densities as shown in the table(3).

Second: Investigate the variation of backscattered count rate with the design parameters as follow:

- **Source – detector separation (Sonde length):**

To investigate the source – detector separation effect on the detected count rate, several runs of Monte Carlo calculation for 10^6 photons in the energy 60 and 662 keV for different densities and the detector is placed at 1,2,3,4 and 5 cm from the source.

The results on figures 4 (a) show that the maximum of total count rate is related to the source – detector separation 2 and 3 on energy 662 keV but on energy 60 keV the maximum count in source – detector separation 1 or 2 except CH_3OH who has the same behavior on both energies because of its high mass attenuation.

- **Energy:**

To determine the optimal source energy for 10^6 photons, different densities and fixed source – detector separation 3 cm, taking range of energies from 50, 100, 200, 300, ……..to 1500 keV.

Figures 5 (a) and (b) shows that most of the materials under investigation have the same shape single peak at about 100 or 200 keV.

The attenuation of gamma rays by photoelectric interaction dominates at energies less than about 140 keV. At higher energies, the contribution of the photons attenuated by scattering is more obvious, especially for energies higher than 200 keV that shows a rapid fall in the count rate.

From this we can conclude that to make an accurate measurement, where the dominant interaction is Compton scattering and to reduce the material chemical composition effect, the source energy must be higher than 200 keV.

- **Density:**

For a range of densities 0.1, 0.2, 0.3, 0.4,…, 3 g/cm^3 for all materials, fixed source – detector separation 3 cm and energies 60 and 662 keV, figures 6 (a), (b), (c), and (d) show that the count rate reaches a maximum at some critical densities which depends on source energy. Below this density, the count rate falls due to the reduced concentration of electrons to scatter photons into the detector. Above this density, the count rate falls due to the increased attenuation of the source beam.

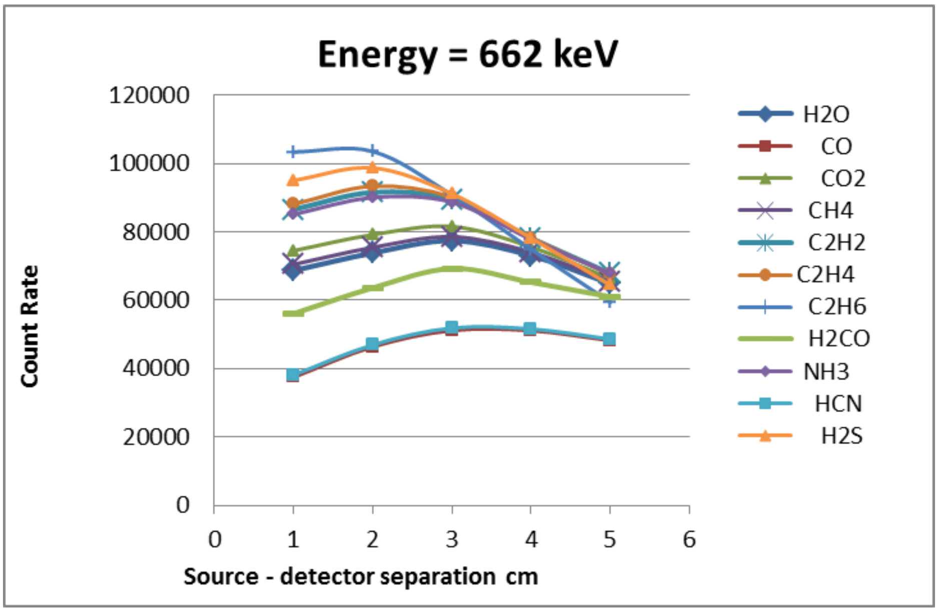
- **Composition:**

To test the effect of chemical composition in more details, several simulation were performed for all the nucleus materials in source – detector separation 1 cm, energy 60 keV and different detector radius (2.5, 5.5, 7.5, 9.5, 12.5 cm).

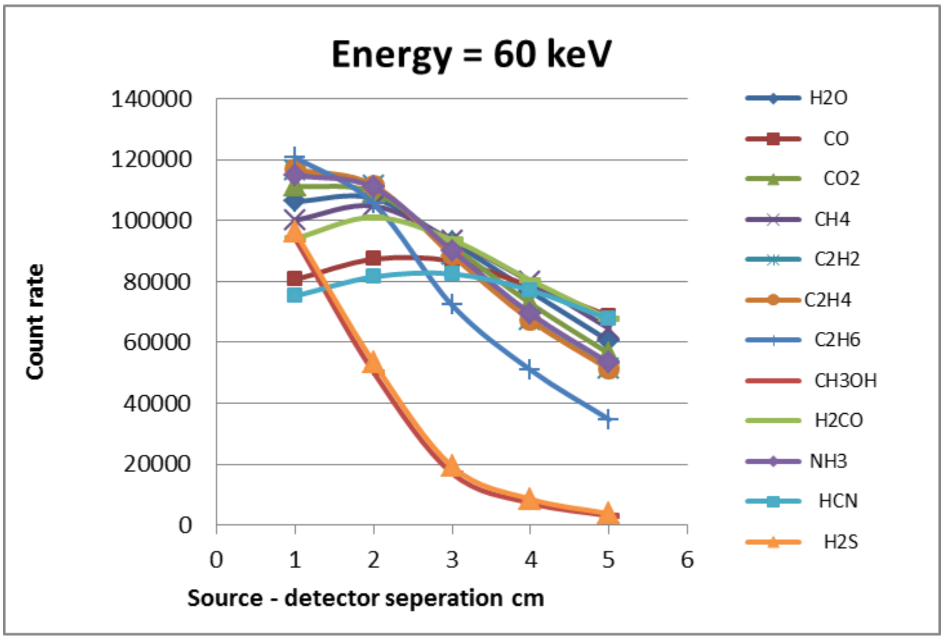
Photoelectric absorption by high Z elements can reduce the count rate but the cometary materials have low Z volatiles.

Table 3- Calculated bulk density of Halley's materials with their real density

Material	Real density (g/cm^3)	Calculated bulk density (g/cm^3)	Sonde length cm
H_2O	0.917	0 .87729	3
CO	0.789	0. 93495	5
CO_2	1.562	1.3742	3
CH_4	0.442	0. 41303	3
C_2H_2	0.729	0 .75186	2
C_2H_4	0.567	0 .56992	2
C_2H_6	0.546	0 .57270	1
CH_3OH	0.791	0 .47224	1
H_2CO	0.815	0.79470	4
NH_3	0.817	0.86260	2
HCN	0.697	0.81737	5
H_2S	1.540	1. 3833	2

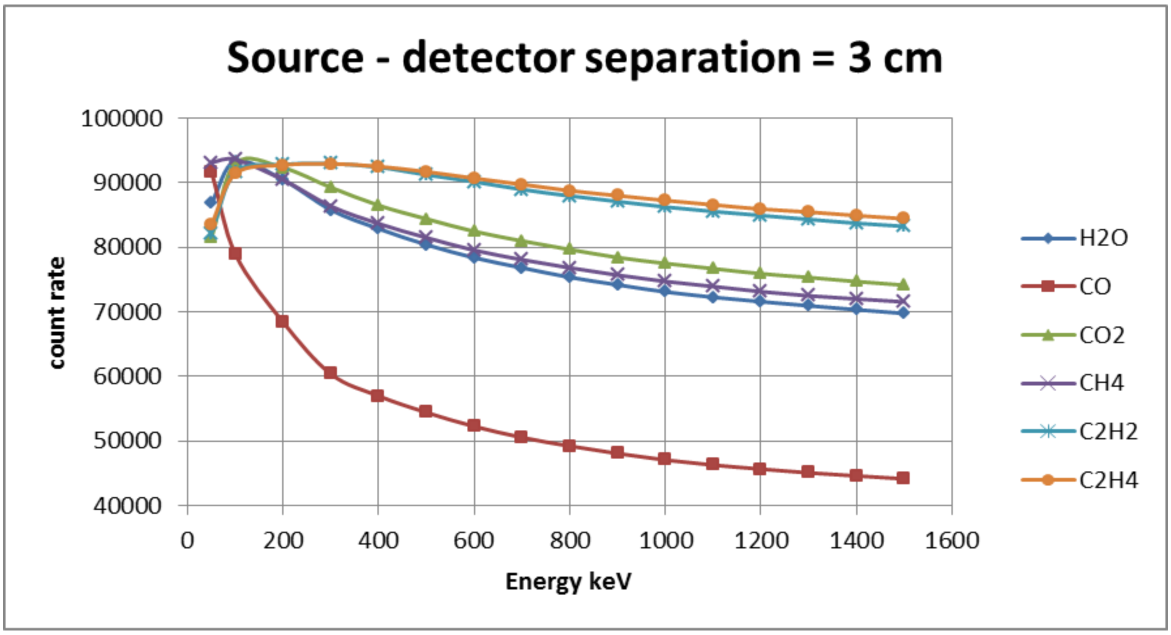


(a)

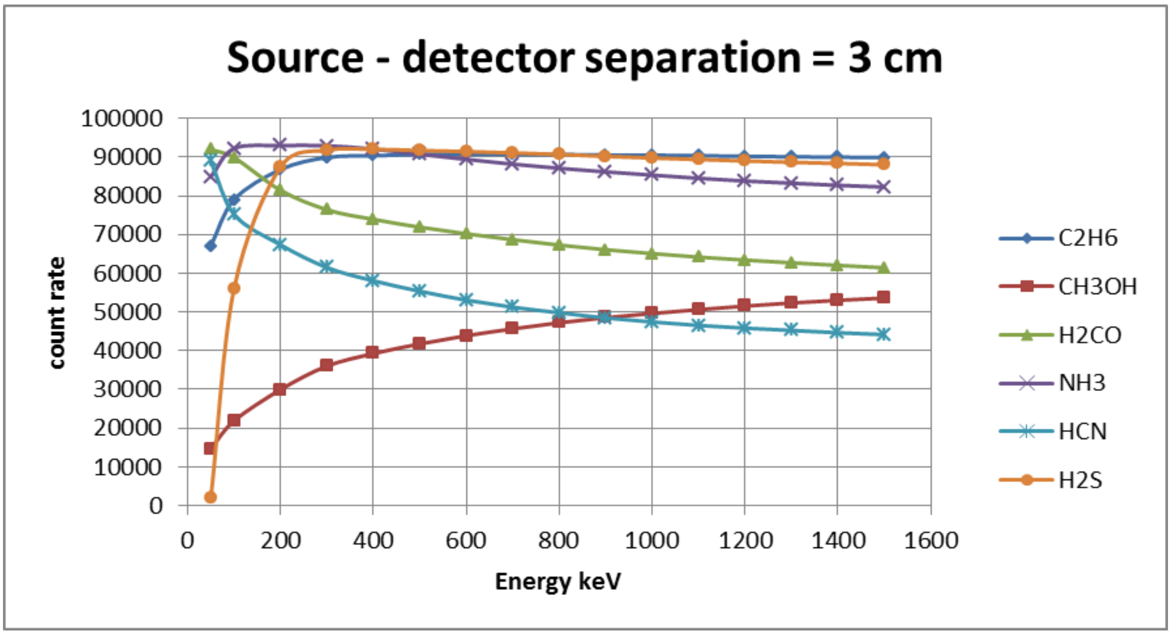


(b)

Figure 4-(a) The count rate vs. source detector separation on energy 662 keV. (b) The count rate vs. source detector separation on energy 60 keV.

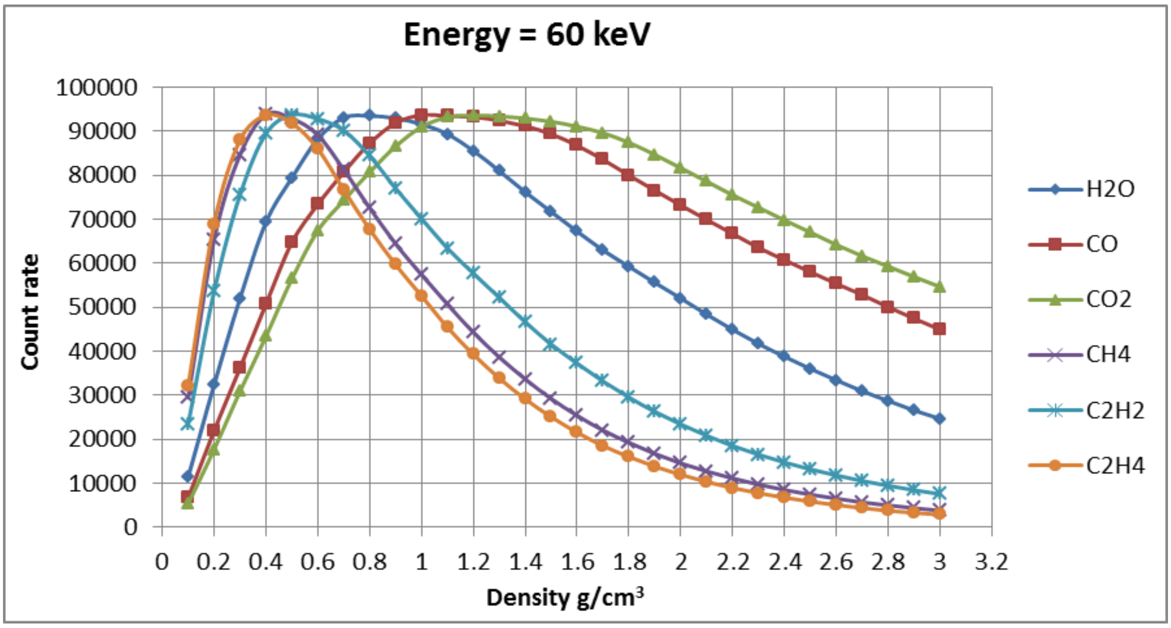


(a)

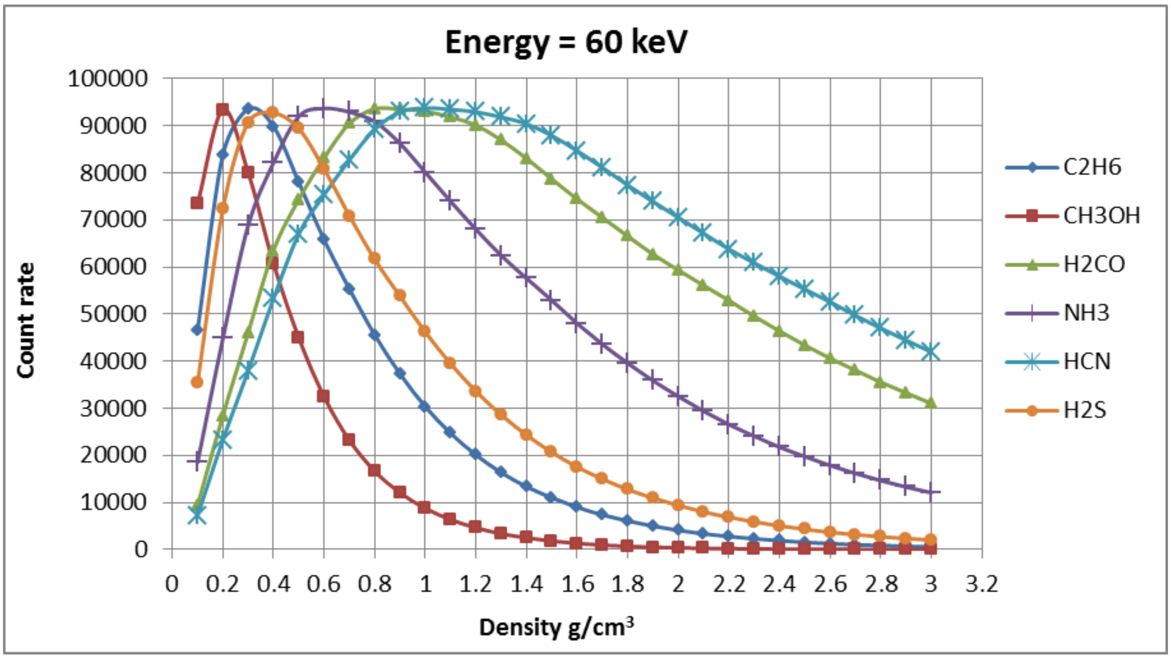


(b)

Figure 5- (a) and (b) The count rate vs. energy (keV) with fixed source – detector separation 3 cm


Energy = 60 keV
Count rate
Density g/cm3
H2O
CO
CO2
CH4
C2H2
C2H4
0
10000
20000
30000
40000
50000
60000
70000
80000
90000
100000
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2

(a)


Energy = 60 keV
Count rate
Density g/cm3
C2H6
CH3OH
H2CO
NH3
HCN
H2S
0
10000
20000
30000
40000
50000
60000
70000
80000
90000
100000
0
0.2
0.4
0.6
0.8
1
1.2
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2
2.2
2.4
2.6
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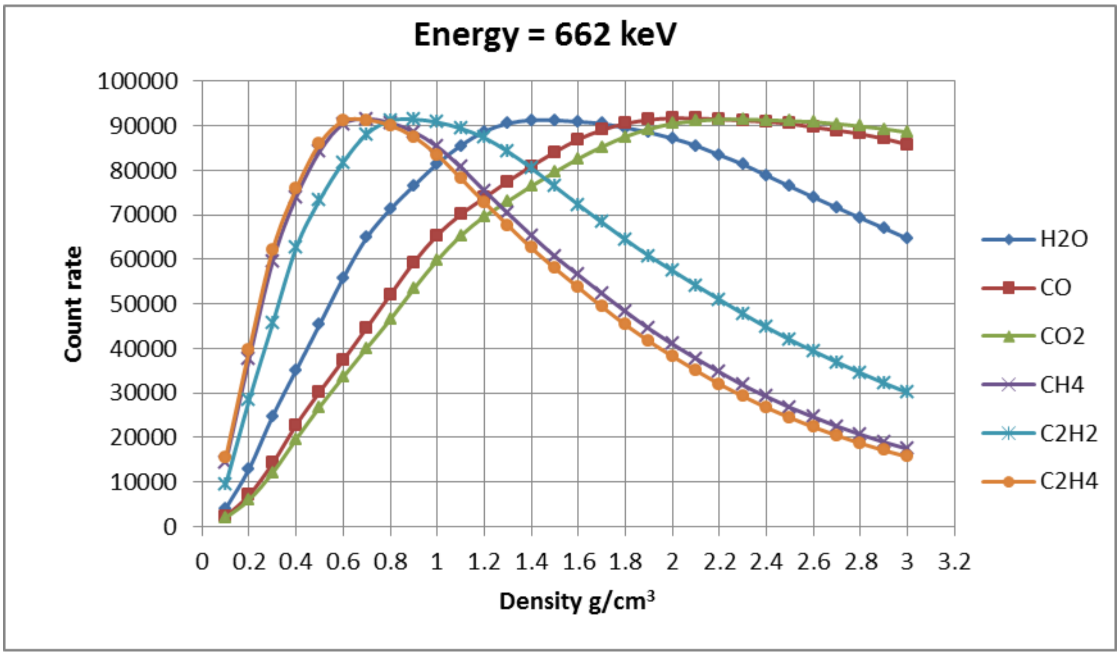
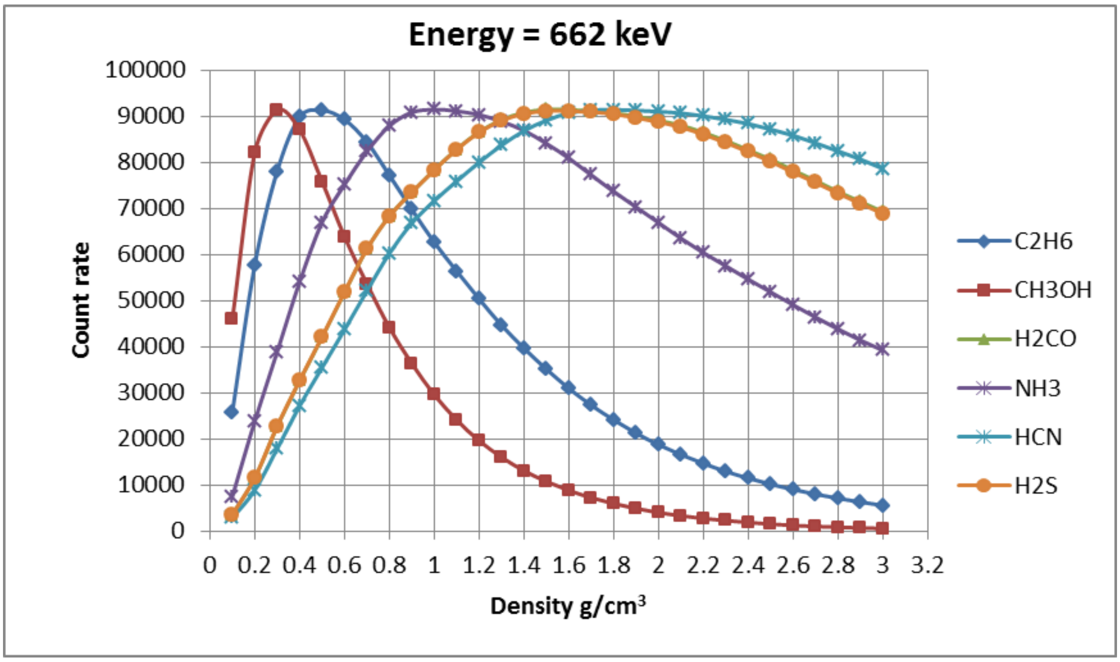
3
3.2

(b)

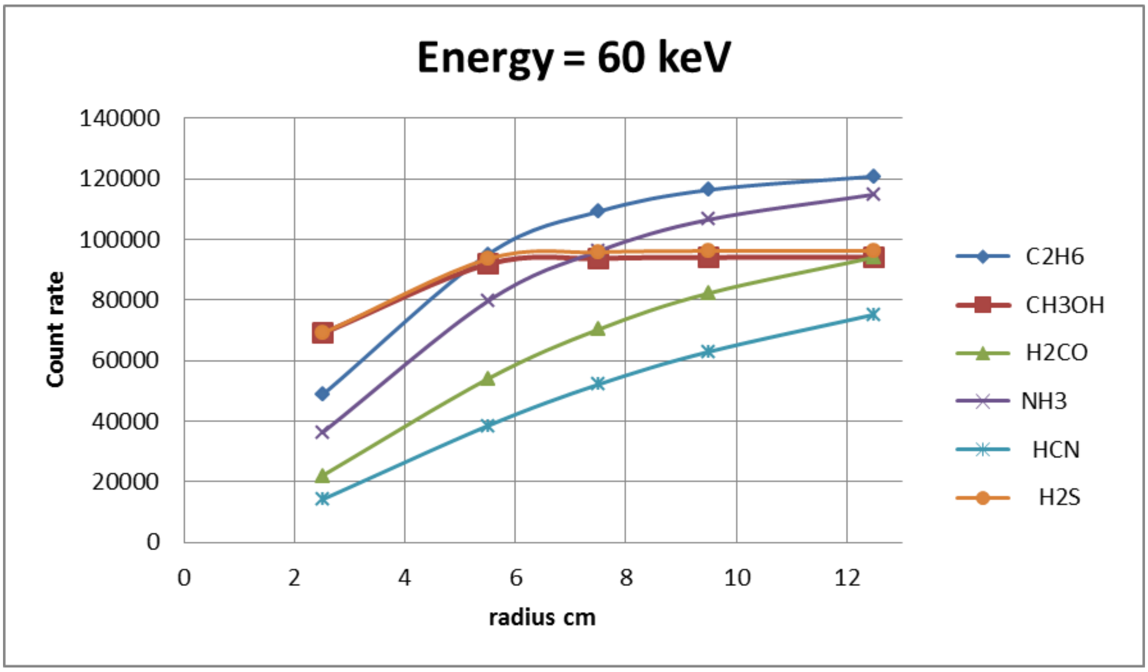


(c)

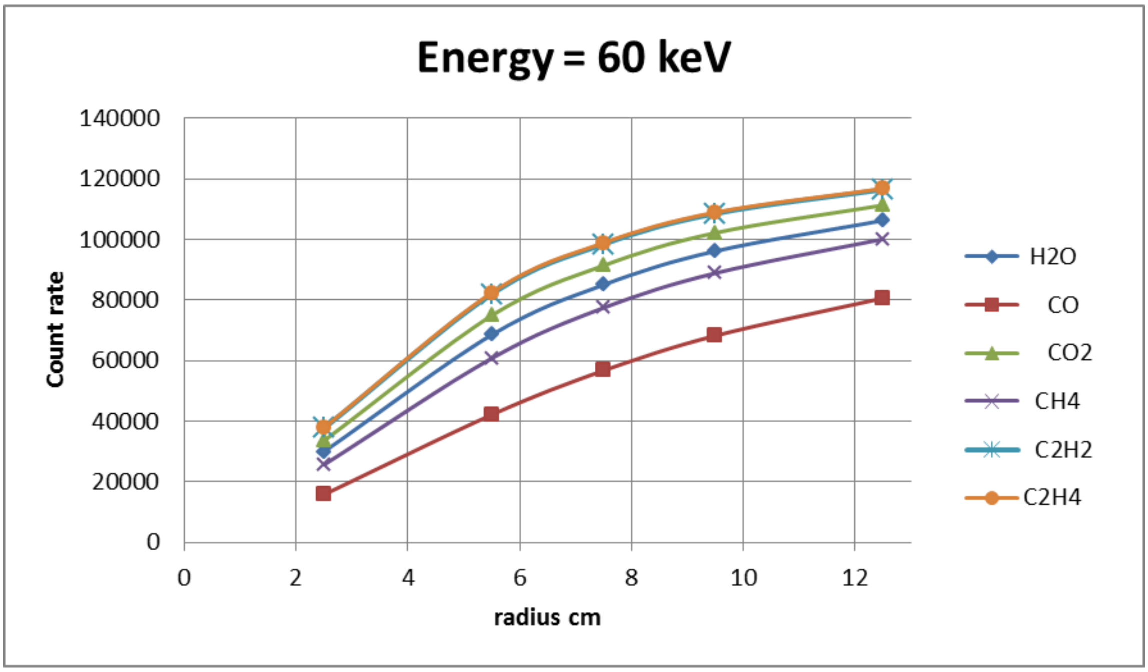


(d)

Figure 6- The count rate vs. density (g/cm^3) in source – detector separation 3 cm. (a) and (b) energy = 60 keV. (c) And (d) energy = 662 keV.



(a)



(b)

Figure 7- (a) and (b) The count rate vs. radius (cm) of the detector with energy 60 keV and fixed source – detector separation 1 cm.

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