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Comparison of calculated spectra for the interaction of photons in a liquid scintillator. Example of ^{54}Mn 835 keV emission

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Abstract

The CIEMAT/NIST and TDCR methods in liquid scintillation counting, initially developed for the activity standardization of pure-beta radionuclides, have been extended to the standardization of electron capture and beta–gamma radionuclides. Both methods require the calculation of the energy spectrum absorbed by the liquid scintillator. For radionuclides emitting X-rays or γ-rays, when the energy is greater than a few tens of keV the Compton interaction is important and the absorption is not total. In this case, the spectrum absorbed by the scintillator must be calculated using analytical or stochastic models. An illustration of this problem is the standardization of ^{54}Mn, which is a radionuclide decaying by electron capture. The gamma transition, very weakly converted, leads to the emission of an 835 keV photon. The calculation of the detection efficiency of this radionuclide requires the calculation of the energy spectrum transferred to the scintillator after the absorption of the gamma ray and the associated probability of absorption. The validity of the method is thus dependent on the correct calculation of the energy transferred to the scintillator.

In order to compare the calculation results obtained using various calculation tools, and to provide the metrology community with some information on the choice of these tools, the LS working group of the ICRM organised a comparison of the calculated absorbed spectra for the 835 keV photon of ^{54}Mn. The result is the spectrum of the energy absorbed by the scintillator per emission of an 835 keV gamma ray. This exercise was proposed for a standard 20 ml LS glass vial and for LS cocktail volumes of 10 and 15 ml. The calculation was done for two different cocktails: toluene and a widely used commercial cocktail, Ultima Gold®. The paper describes the results obtained by nine participants using a total of 12 calculation codes.

Keywords: Liquid scintillator; Photon interactions; ^{54}Mn

1. Introduction

In liquid scintillation counting, the CIEMAT/NIST and TDCR methods, initially developed for the activity standardization of pure-beta radionuclides, have been extended to the standardization of electron capture radionuclides or beta–gamma radionuclides. Both methods are based on the same physical and statistical models and the calculation of the detection efficiency requires the calculation of the energy spectrum absorbed by the liquid scintillator.

For pure-beta or low-Z pure electron capture radionuclides, the calculation of the absorbed spectrum is

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straightforward, as it can be assumed that the absorbed spectrum is the emission spectrum. This is not the case for radionuclides emitting X-rays or gamma rays, when the energy is greater than a few tens keV. As the liquid scintillator is a low-Z and low-density material, the Compton interaction is important and the absorption is not total. In this case, the spectrum absorbed by the scintillator must be calculated using analytical or stochastic models. Several models were specifically developed for this purpose but general purpose Monte Carlo radiation–matter interaction software, like MCNP, EGS, GEANT or PENELOPE can also be used.

A practical example where this kind of problem is encountered is the standardization of ^{54}Mn, a radionuclide decaying through electron capture towards an excited level of ^{54}Cr. The gamma transition is very weakly converted and leads to the emission of an 835 keV photon. The calculation of the detection efficiency of this radionuclide using the CIEMAT/NIST or the TDCR method requires the calculation of the energy spectrum transferred to the scintillator by the absorption of the gamma ray and the associated probability of absorption. The validity of the method is thus dependent on the correct calculation of the energy transferred to the scintillator.

In order to compare the calculation results obtained using various calculation tools, and to provide the metrology community with some information on the choice of these tools, the LS working group of the ICRM organised a comparison of the calculated absorbed spectra for the 835 keV photon of ^{54}Mn. In this calculation, only the gamma emission was considered (i.e. the X-ray and Auger electrons emitted following the capture and the weak electron conversion process are not taken into account). This paper explains this exercise and the results obtained.

2. Description of the exercise

The anticipated results are the spectrum of the energy absorbed by the scintillator per emission of an 835 keV gamma ray. The characteristics of this spectrum are also indicated by two parameters: the integral of this spectrum, which is the probability of interaction of the 835 keV gamma ray within the LS cocktail, and the average energy deposited in the scintillator per gamma ray emitted.

This exercise was proposed for a standard 20 ml LS glass vial and for LS cocktail volumes of 10 and 15 ml. A preliminary calculation was proposed, considering only a cylinder of LS cocktail, without any surrounding material and in the vacuum. The purpose of this preliminary calculation, described in Fig. 1, was to test the simple absorption model and to check that there was nothing wrong in the cross section used.

The other calculations concern 10 and 15 ml volumes of two LS cocktails in a 20 ml glass vial surrounded by a simplified counting chamber structure. All geometries can be described by coaxial cylinders. The dimensions of the vial filled with 10 and 15 ml of LS are given in Figs. 2 and 3. The calculation is done for two different cocktails: toluene and a widely used commercial cocktail, Ultima Gold®

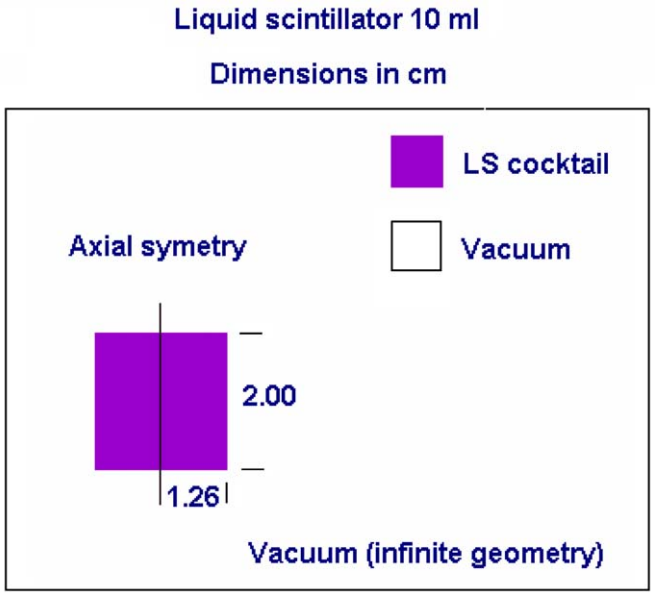

Fig. 1. Preliminary calculation: cylinder of 10 ml of LS cocktail in vacuum (infinite geometry).

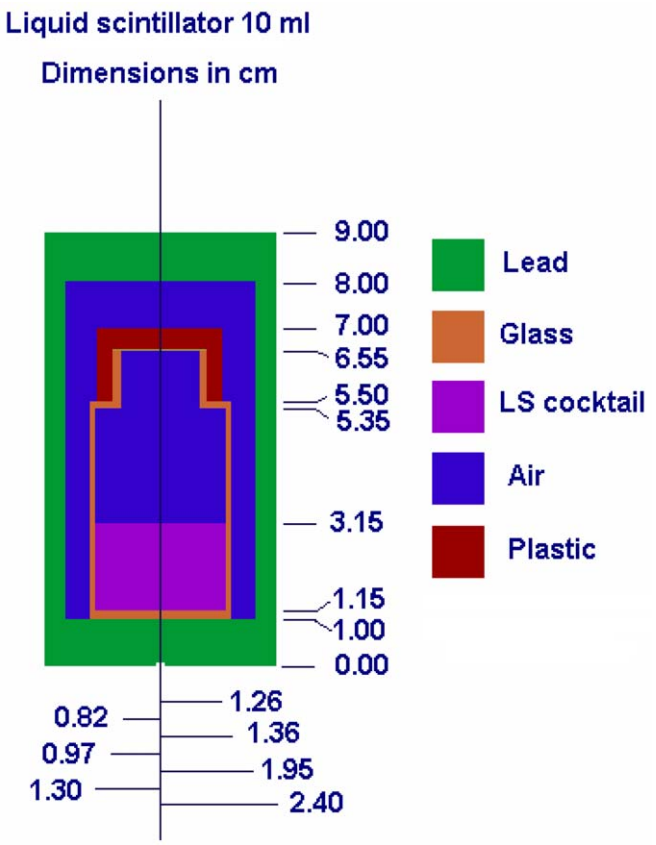

Fig. 2. LS cocktail, 10 ml in a LS vial inside a LS counter.

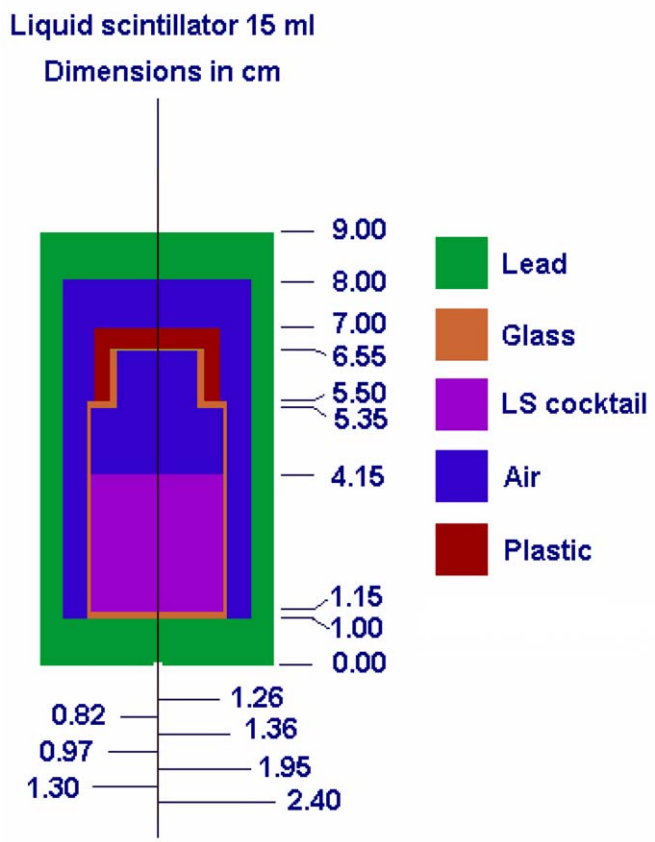

Fig. 3. LS cocktail, 15 ml in a LS vial inside a LS counter.

Table 1
Stoichiometric formula and density of the scintillators

	C	H	N	O	P	S	Na	Density at 20 °C (g/cm^3)
Toluene	7	8						0.87
Ultima Gold	16.81	24.54	0.040	1.52	0.11	0.02	0.02	0.98

(Perkin Elmer). The atomic composition and density of the cocktails are given in Table 1.

The exercise started at the end of June 2004 and the results were collected at the end of January 2005.

3. Participants

The proposal to participate in this exercise was sent to a mailing list of people attending the ICRM LSCWG business meeting in May 2003 in Dublin. The coordinator received 17 answers from people interested in participating and, eventually, nine teams from eight laboratories completed the exercise. These laboratories are: IAEA (International organization); CIEMAT (Spain), two answers from different teams; CSIR-NML (South Africa); IRA-METAS (Switzerland); IRMM (European Commission); KRISS (Republic of Korea); LNHB (France); PTB (Germany).

Some participants used general-purpose Monte Carlo simulation codes and others used locally developed (LD) codes. The codes used are: PENELOPE (Salvat et al., 2003); MCNPX (University of California, 1998, 2003); MCNP4 C2 (Briesmeister, 2000); GEANT3 (Brun et al., 1987; CERN, 2005); EGS-NRC (Nelson et al., 1985; Kawrakow, 2000; Kawrakow et al., 2003).

The locally developed codes are: GEOLEP (Solé, 1990; Solé and Denecke, 1992); EMILIA (Malonda et al., 1994; Carles, 2006); PTB (PTB), (Kossert, 2005); SOBEGA (Torano, 1998); MONTY (Simpson, 1994).

Some participants used more than one code and a total of 12 calculations were analysed.

A summary of the results reported is described hereafter.

4. Simulation of toluene

4.1. 10 ml of LS without surrounding material

This first calculation concerned a cylinder of pure toluene without vial or surrounding structure. The purpose of this first test (although physically unrealistic) was to compare a simple absorption model and to check the consistency of the cross section used. The results are summarized in Table 2, where mean values and standard deviation of the absorption probability and of the average absorbed energy are calculated. It must be pointed out that these mean values are not weighted by the claimed uncertainties or by the number of photons simulated. For 12 results, the relative standard deviation of the absorption probabilities is 1.1% and the relative standard deviation of the average energy absorbed is 3.0%.

4.2. 10 ml of LS with vial and surrounding materials

The calculation is similar to the one described in 4.1 but with a model of the vial and the counting chamber. The results are summarized in Table 3. For nine results, the relative standard deviation of the absorption probabilities is 2.8% and the relative standard deviation of the average energy absorbed is 3.3%.

4.3. 15 ml of LS with vial and surrounding materials

The calculation is the same as in 4.2 but with 15 ml of scintillator. The results are summarized in Table 4. For nine results, the relative standard deviation of the absorption probabilities is 8.7% and the relative standard deviation of the average energy absorbed is 9.2%. If the result 8b is not considered, these relative standard deviations become 3.1% and 3.4%, respectively.

4.4. Effect of surrounding material and volume

The effect of surrounding material on the absorption probability and on the average energy for toluene is

Table 2
Simulation of toluene without vial and surrounding materials

Laboratory	Code name	No. of photons simulated	Probability of absorption (%)	Standard uncertainty	Average energy absorbed per photon (keV)	Standard uncertainty on the energy (keV)	Absorption coefficient (cm^{-1})
1	EGS-NRC-MP	2×10^6	6.14	0.17	20.15	0.066	
1bis	PENELOPE 3	2×10^6	6.09	0.16	19.956	0.200	6.56×10^{-2}[a]
2	LD1	4×10^6	6.23	0.20	21.9		
3	PENELOPE 3	5.9×10^6	6.18	0.01	20.29	0.12	6.76×10^{-2}
3b	MCNPX 2.5d3	5×10^6	6.17	0.01	20.19	0.03	
4	GEANT 3	9.42×10^8	6.35	0.01	21.20	0.02	6.68×10^{-2}
5	LD2	5×10^7	6.19		20.38[b]		6.63×10^{-2}
6	MCNP 4c2	1×10^7	6.2		20.21[b]		
7	LD3	2.5×10^6	6.10	0.17	20.34[b]		6.69×10^{-2}[c]
8	LD4	5×10^6	6.22		21.89[b]		6.66×10^{-2}
8b	PENELOPE	5×10^6	6.19		19.99[b]		6.55×10^{-2}
9	LD5	1×10^7	6.12		21.9		6.55×10^{-2}
Average			6.182		20.70		6.50×10^{-2}
Standard deviation			0.070		0.79		0.43×10^{-2}

[a]Calculated from 1.157×10^{-23} cm^2 reported by the laboratory, using a density of 0.87 for toluene.
[b]Calculated by the coordinator as the average energy per interaction multiplied by the absorption probability.
[c]Calculated from 0.0769 $cm^2 g^{-1}$ reported by the laboratory.

Table 3
Simulation of 10 ml of toluene in a glass vial with surrounding materials

Laboratory	Code name	No. of photons simulated	Probability of absorption (%)	Standard uncertainty	Average energy absorbed per photon (keV)	Standard uncertainty on the energy (keV)
1	EGS-NRC-MP	2×10^6	6.50	0.17	20.870	0.063
1bis	PENELOPE 3	2×10^6	6.49	0.17	20.835	0.020
2	LD1					
3	PENELOPE 3	4.5×10^6	6.49	0.01	20.79	
3b	MCNPX 2.5d3	5×10^6	6.71	0.01	21.55	0.04
4	GEANT 3	9.42×10^8	6.59	0.01	21.400	0.002
5	LD2					
6	MCNP 4c2	1×10^7	6.5		20.67[a]	
7	LD3					
8	LD4					
8b	PENELOPE	5×10^6	6.25		20.13[a]	
9	LD5	1×10^7	6.24		22.4	
Average			6.47		21.08	
Standard deviation			0.16		0.69	

[a]Calculated by the coordinator as the average energy per interaction multiplied by the absorption probability.

summarized in Figs. 4 and 5. The effect of volume is presented in Figs. 6 and 7.

5. Simulation of Ultima Gold

5.1. 10 ml of LS without surrounding material

The calculation is similar to the one described in 4.1. The results are summarized in Table 5. For 12 results, the relative standard deviation of the absorption probabilities is 3.8% and the relative standard deviation of the average energy absorbed is 3.7%. If the result nine is not considered, these relative standard deviations become, respectively, 1.3% and 3.6%.

5.2. 10 ml of LS in a glass vial with surrounding material

The calculation is similar to the one described in 5.1 but with a model of the vial and the counting chamber. The results are summarized in Table 6. For nine results, the

Table 4
Simulation of 15 ml of toluene in a glass vial with surrounding materials

Laboratory	Code name	No. of photons simulated	Probability of absorption (%)	Standard uncertainty	Average energy absorbed per photon (keV)	Standard uncertainty on the energy (keV)
1	EGS-NRC-MP	2×10^6	7.61	0.19	24.79	0.069
1bis	PENELOPE 3	2×10^6	7.42	0.19	24.20	0.022
2	LD1					
3	PENELOPE 3	4.4×10^6	7.32	0.01	23.74	0.15
3b	MCNPX 2.5d3	5×10^6	7.59	0.01	24.74	0.04
4	GEANT 3	9.42×10^8	7.46	0.01	24.600	0.002
5						
6	MCNP 4c2	1×10^7	7.3		23.51[a]	
7	LD3					
8	LD4					
8b	PENELOPE	5×10^6	9.22		30.70[a]	
9	LD5	1×10^7	7.06		25.4	
Average			7.62 (7.39[b])		25.2 (24.43[b])	
Standard deviation			0.67 (0.19[b])		2.3 (0.65[b])	

[a]Calculated by the coordinator as the average energy per interaction multiplied by the absorption probability.
[b]Without result 8b.

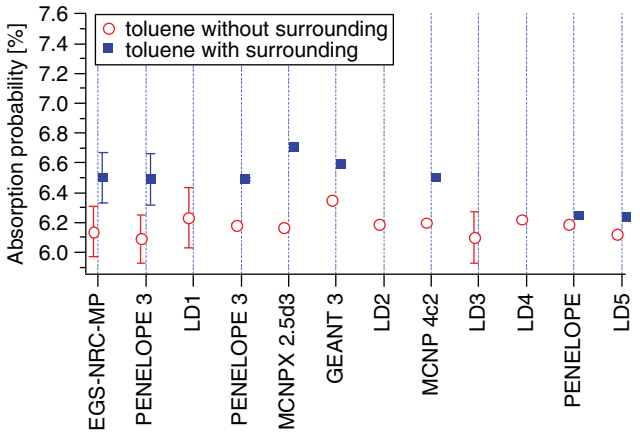

Fig. 4. Absorption probability: toluene 10 ml with and without surrounding material.

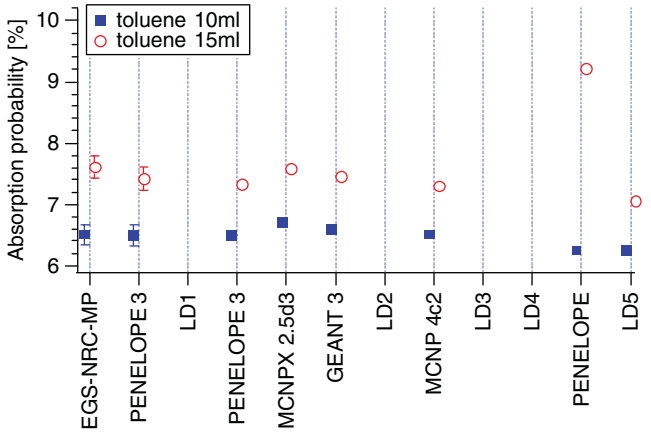

Fig. 6. Effect of volume on the absorption probability, toluene.

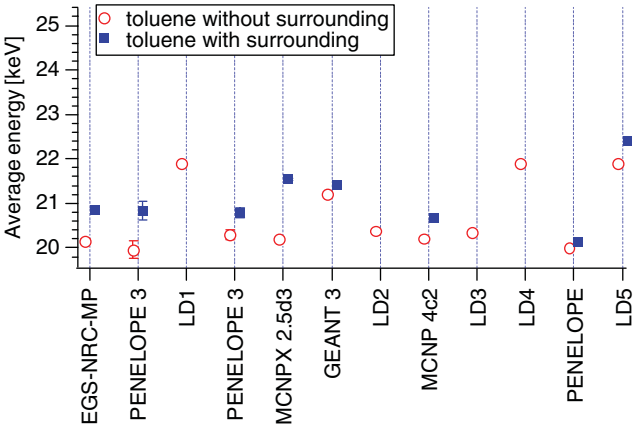

Fig. 5. Average energy: toluene 10 ml with and without surrounding material.

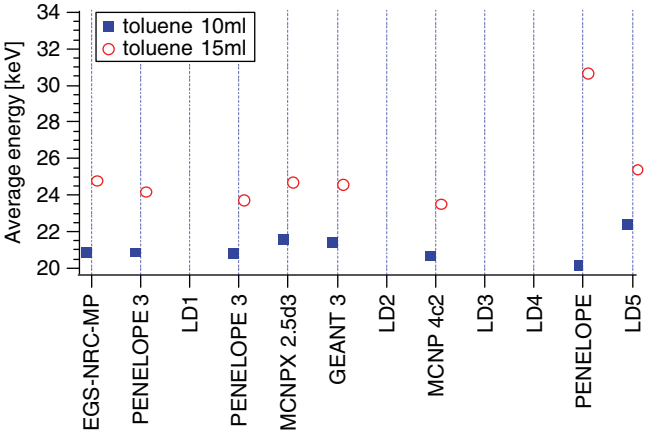

Fig. 7. Effect of volume on the average energy, toluene.

Table 5
Simulation of 10 ml of Ultima Gold without glass vial and surrounding materials

Laboratory	Code name	No. of photons simulated	Probability of absorption (%)	Standard uncertainty	Average energy absorbed per photon (keV)	Standard uncertainty on the energy (keV)	Absorption coefficient (cm^{-1})
1	EGS-NRC-MP	2×10^6	6.92	0.18	23.02	0.071	
1bis	PENELOPE 3	2×10^6	6.89	0.16	22.94	0.021	7.50×10^{-2}[a]
2	LD1		7.08	0.20	25.0		
3	PENELOPE 3	5.2×10^6	6.90	0.01	22.95	0.13	7.58×10^{-2}
3b	MCNPX 2.5d3	5×10^6	6.89	0.01	22.83	0.04	
4	GEANT 3	9.42×10^8	7.08	0.01	23.900	0.002	7.49×10^{-2}
5	LD2	5×10^7	6.90		22.58[b]		7.43×10^{-2}
6	MCNP 4c2	1×10^7	6.9		22.77[b]		
7	LD3	2.5×10^6	6.89	0.21	22.55[b]		7.59×10^{-2}[c]
8	LD4	5×10^6	7.14		25.28[b]		7.60×10^{-2}
8b	PENELOPE	5×10^6	6.98		22.96[b]		7.44×10^{-2}
9	LD5	1×10^7	6.15		22.0		7.42×10^{-2}
Average			6.89		23.23		7.25
Standard deviation			0.25		0.99		0.76

[a]Calculated from $3.2512 \times 10^{-23}\,cm^2$ reported by the laboratory, using Ultima Gold atomic mass of 255.76 and density of 0.98.
[b]Calculated by the coordinator as the average energy per interaction multiplied by the absorption probability.
[c]Calculated from $0.0769\,cm^2\,g^{-1}$ reported by the laboratory.

Table 6
Simulation of 10 ml of Ultima Gold in a glass vial with surrounding materials

Laboratory	Code name	No. of photons simulated	Probability of absorption (%)	Standard uncertainty	Average energy absorbed per photon (keV)	Standard uncertainty on the energy (keV)
1	EGS-NRC-MP	2×10^6	7.37	0.18	23.99	0.068
1bis	PENELOPE 3	2×10^6	7.39	0.18	23.99	0.022
2	LD1					
3	PENELOPE 3	3.2×10^6	7.20	0.02	23.39	0.17
3b	MCNPX 2.5d3	5×10^6	7.47	0.01	24.31	0.04
4	GEANT 3	9.42×10^8	7.34	0.01	24.100	0.002
5	LD2					
6	MCNP 4c2	1×10^7	7.2		23.18[a]	
7	LD3					
8	LD4					
8b	PENELOPE	5×10^6	7.05		23.12[a]	
9	LD5	1×10^7	7.04		25.3	
Average			7.26		23.92	
Standard deviation			0.16		0.71	

[a]Calculated by the coordinator as the average energy per interaction multiplied by the absorption probability.

relative standard deviation of the absorption probabilities is 2.6% and the relative standard deviation of the average energy absorbed is 3.4%.

5.3. 15 ml of LS in a glass vial with surrounding material

The calculation is the same as in 5.2 but with 15 ml of scintillator. The results are summarized in Table 7. For nine results, the relative standard deviation of the absorption probabilities is 8.1% and the relative standard deviation of the average energy absorbed is 8.8%. If the result 8b is not considered, these relative standard deviations become 4.1% and 7.7%, respectively.

5.4. Effect of surrounding material and volume

The effect of surrounding material on the absorption probability and on the average energy for toluene is summarized in Figs. 8 and 9. The effect of volume is presented in Figs. 10 and 11.

6. Comparison of spectra

A typical interaction spectrum can be observed in Fig. 12. This spectrum shows a clear Compton edge, with a little structure in the high-energy region, which can be attributed to double and multiple Compton interactions. It

Table 7
Simulation of 15 ml of Ultima Gold in a glass vial with surrounding materials

Laboratory	Code name	No. of photons simulated	Probability of absorption (%)	Standard uncertainty	Average energy absorbed per photon (keV)	Standard uncertainty on the energy (keV)
1	EGS-NRC-MP	2×10^6	8.59	0.20	28.400	0.074
1bis	PENELOPE 3	2×10^6	8.86	0.19	29.491	0.024
2	LD1					
3	PENELOPE 3	3×10^6	8.16	0.02	26.77	0.19
3b	MCNPX 2.5d3	5×10^6	8.45	0.01	27.87	0.04
4	GEANT 3	9.42×10^8	8.31	0.01	27.700	0.003
5	LD2					
6	MCNP 4c2	1×10^7	8.2		26.81[a]	
7	LD3					
8	LD4					
8b	PENELOPE	5×10^6	10.11		34.07[a]	
9	LD5	1×10^7	7.97		28.8	
Average			8.58 (8.36[b])		28.7 (28.0[b])	
Standard deviation			0.68 (0.30[b])		2.4 (1.0[b])	

[a]Calculated by the coordinator as the average energy per interaction multiplied by the absorption probability.
[b]Without result 8b.

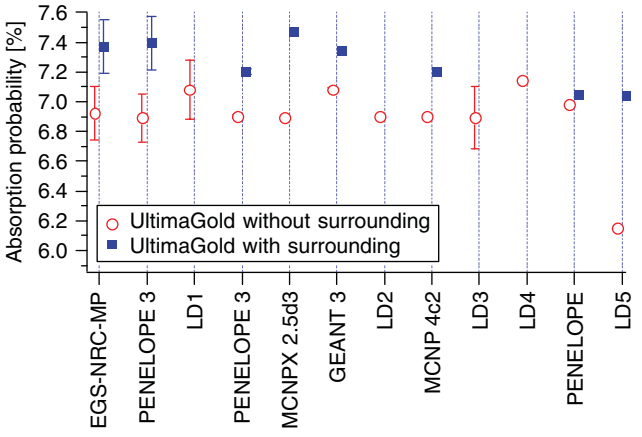

Fig. 8. Absorption probability: Ultima Gold 10 ml with and without surrounding material.

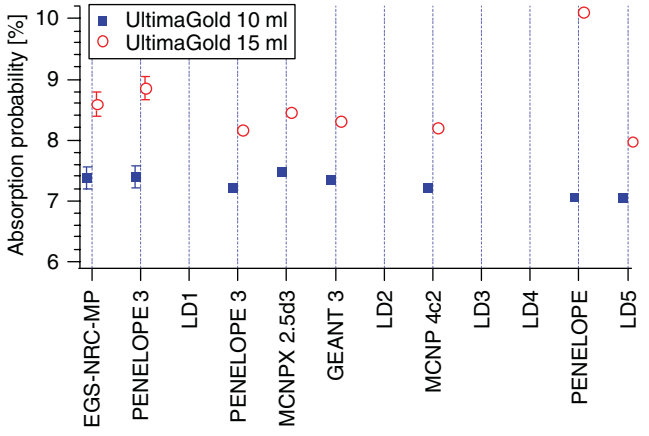

Fig. 10. Effect of volume on the absorption probability, Ultima Gold.

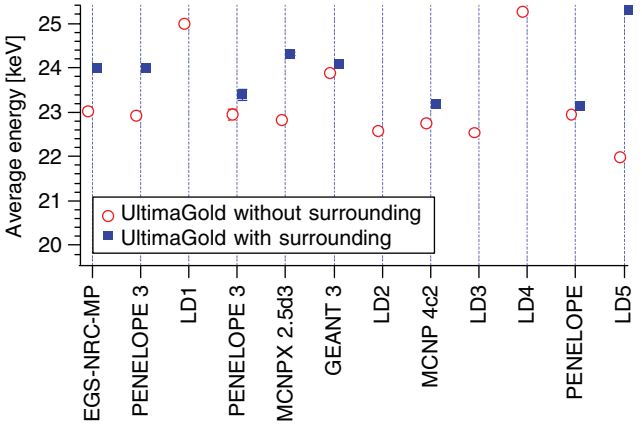

Fig. 9. Average energy: Ultima Gold 10 ml with and without surrounding material.

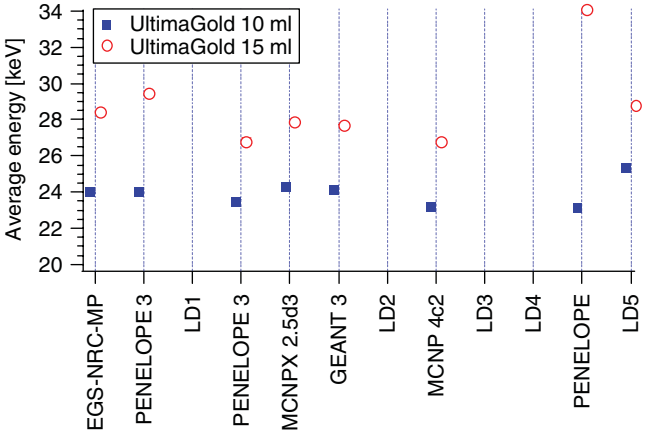

Fig. 11. Effect of volume on the average energy, Ultima Gold.

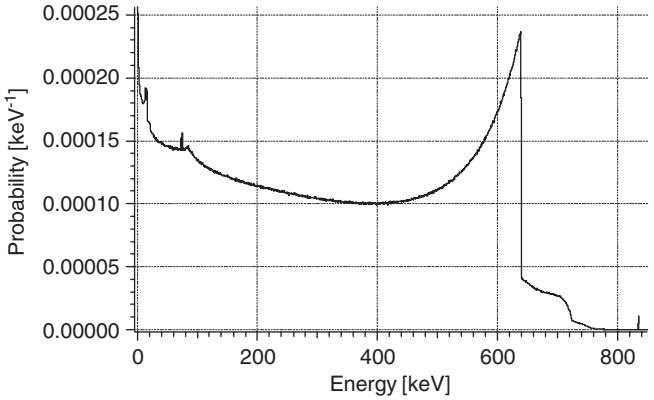

Fig. 12. Typical interaction spectrum.

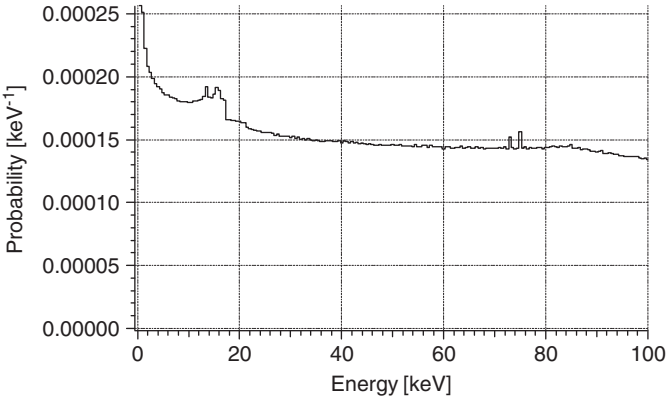

Fig. 13. Low-energy part of the spectrum calculated by GEANT3.

must be observed that laboratories nos. 5 and 7 did not add the energy of multiple Compton interactions to the main Compton spectrum. This can be explained because, as the calculation tool used is devoted to liquid scintillation studies, it is necessary to separate multiple coincident events, as the energy is not additive due to the non-linearity of the scintillator. In this problem the ratio of the area of multiple Compton peaks to the area of the total spectrum is about 2.2%.

In order to compare the calculated spectra we present in Table 10 some characteristics of the shape of the spectra, namely, the peak-to-valley ratio of the main Compton spectrum and the ratio of the amplitude of the multiple Compton peak to the amplitude of the main Compton peak. The compared spectra are relative to the simple toluene calculation without vial and counter structures.

In the spectra calculated considering the vial and the counter structures, the low-energy part of the spectrum is generally more important because of diffusion but, in most cases, the general shape of the spectrum remains similar to the one calculated without structures. With spectra calculated with high statistics, discrete structures are present in the lower energy part of the spectrum as shown in Fig. 13, the spectrum calculated using GEANT 3 for almost 10^9 photons. These structures are probably due to the X-ray fluorescence of the lead of the counter structure, absorbed by the LS cocktail.

7. Discussion

The minimum dispersion between the results is around 1% and is obtained in the simplest calculation case, i.e. 10 ml of toluene without vial and counter structures. The dispersion becomes more important, higher than 8%, with 15 ml of scintillator for both toluene and Ultima Gold when vial and surrounding structures are taken into account.

The dispersion of the absorption coefficients is about 7% for toluene and more than 10% for Ultima Gold. At first glance, this could explain the dispersion in the results but it happens that there is no obvious correlation between the absorption coefficients and the absorption probabilities. For example, in Table 2, the results no. 5 and 8b are similar but the relative difference of the absorption coefficients is about 20%.

Table 8 and Figs. 14 and 15 show the increase of the absorption probability and average absorbed energy when vial and structure are considered. For the absorption probability, this relative increase is between 1% and 8.8% for toluene and between 1% and 15% for Ultima Gold. For the average energy absorbed, this range is 0.7–6.7% for toluene and 0.7–6.5% for Ultima Gold. From all results considered, it seems that the modelling of the vial and of the counter structure cannot be neglected. Even though the fluctuations between calculations are high, all results show that the modelling of the vial and of the structure increases the interaction probability and average energy.

The code PENELOPE was employed by three of the participants and it was interesting to compare the results. The probabilities of absorption calculated using PENELOPE for each case are summarized in Table 9, and the standard deviation of the results is compared with the standard deviation of all the results. It happens that, except for the case of Ultima Gold without vial and structures, the standard deviation between the results calculated with PENELOPE are similar or even greater than the standard deviation of all the results. Although it is quite difficult to draw a general conclusion, it seems that the variation from laboratory to laboratory is higher than from code to code (Table 10).

The calculation of the spectrum corresponding to the absorption of the gamma ray is only a part of the calculation of the detection efficiency of ^{54}Mn in LSC using CIEMAT/NIST or TDCR methods. Other phenomena must be considered important, namely the scintillator non-linearity (ionization quenching), the probability of absorption of X-rays in the scintillator and the detailed description of the energy released after the electron capture process, including M events. To give an order of magnitude of the importance of the calculation of the gamma ray absorption in the detection efficiency, let us suppose that the detection efficiency of the electron capture branch is

Table 8
Influence of vial and surrounding structures for 10 ml of toluene

Laboratory	Code name	Relative increase in absorption probability (%)	Relative increase in absorption probability (%)	Relative increase in average absorbed energy (%)	Relative increase in average absorbed energy (%)
		Toluene	Ultima Gold	Toluene	Ultima Gold
1	EGS-NRC-MP	+5.9	+6.5	+3.6	+4.2
1bis	PENELOPE 3	+6.6	+7.3	+4.4	+4.6
2	LD1	n.d.	n.d.	n.d.	n.d.
3	PENELOPE 3	+5.0	+4.4	+2.5	+1.9
3b	MCNPX 2.5d3	+8.8	+8.4	+6.7	+6.5
4	GEANT 3	+3.8	+3.7	+0.9	+0.8
5	LD2	n.d.	n.d.	n.d.	n.d.
6	MCNP 4c2	+4.8	+4.4	+2.3	+1.8
7	LD3	n.d.	n.d.	n.d.	n.d.
8	LD4	n.d.	n.d.	n.d.	n.d.
8b	PENELOPE	+1.0	+1.0	+0.7	+0.7
9	LD5	+1.9	+15	+2.3	+15

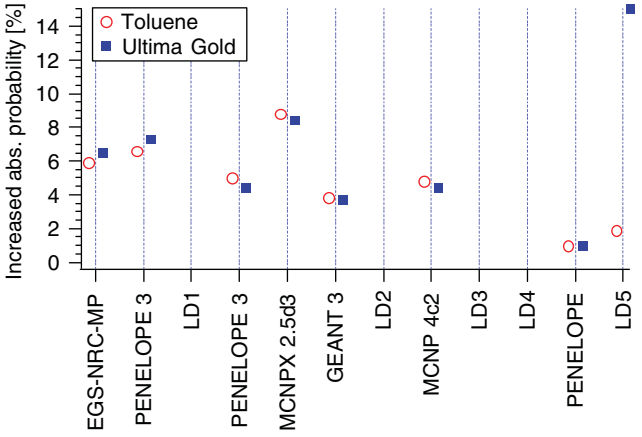

Fig. 14. Effect of surrounding material on the absorption probability.

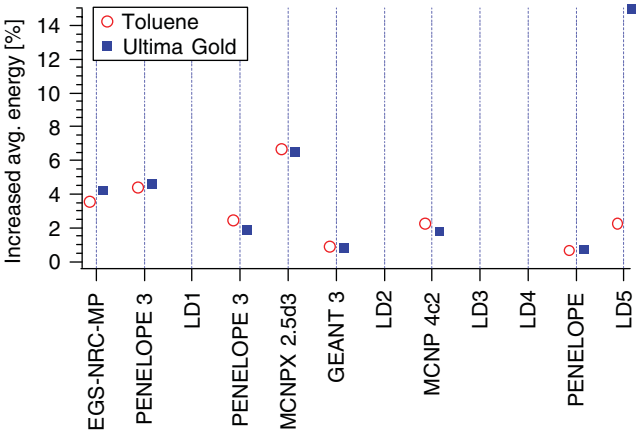

Fig. 15. Effect of surrounding material on the average energy.

about 0.5. This value is realistic for a commercial LSC counter or a 3-PMT counter, as it is approximately the value observed for ^{55}Fe, which decays through electron capture to the fundamental level of manganese. Under this assumption, the global detection efficiency of ^{54}Mn, ε_D, can be written as

$$\varepsilon_D = \varepsilon_\gamma P_\gamma + (1 - P_\gamma) \bullet \varepsilon_{capture}, \quad (1)$$

where ε_γ is the detection efficiency when the gamma ray is absorbed, P_γ is the probability of absorption of the gamma ray and $\varepsilon_{capture}$ is the detection efficiency of the capture branch.

The average energy released per 835 keV photon emission is about 28 keV for 15 ml of scintillator but the average energy deposited when the 835 keV gamma ray interacts with the scintillator is about 330 keV. This means that, the detection efficiency of such event, ε_γ , is likely to be close to 1. If we consider the extreme values of Table 7, P_γ is in the 7.79–8.86% range. With the previous assumption, this gives an ε_D value between 0.539 and 0.544, which is a 0.9% relative increase.

8. Conclusions

The spectrum of the energy transferred in a liquid scintillator after the absorption of an 835 keV gamma ray has been calculated for three standard geometries by nine laboratories. The relative standard deviation of the absorption probability is about 1% for a simple scintillator (toluene) and a simple geometry (isolated LS cocktail without surroundings). For more complex situations (Ultima Gold with vial and counter description), the relative standard deviation is in the 2.6–8.7% range. The largest dispersions are reached for a volume of scintillator of 15 ml, i.e. for the largest absorption probabilities values. In this case, the photon absorption coefficients to consider are not only the values at 835 keV but also the values in the 0–835 keV energy range, because diffusion and fluorescence phenomena are no longer negligible.

Even in the worst case, the absolute standard deviation of the absorption probability remains under 1%. This comparison shows that the contribution of the 835 keV

Table 9
PENELOPE results compared and compared with all results

Laboratory	Probability of absorption (%)	Probability of absorption (%)	Probability of absorption (%)	Probability of absorption (%)	Probability of absorption (%)	Probability of absorption (%)
	10 ml toluene	10 ml toluene with structures	10 ml Ultima Gold	10 ml Ultima Gold with structures	15 ml toluene with structures	15 ml Ultima Gold with structures
1bis	6.09	6.49	6.89	7.39	7.42	8.86
3	6.18	6.49	6.90	7.20	7.32	8.16
8b	6.19	6.25	6.98	7.05	9.22	10.11
Relative standard deviation (%)	0.9%	2.2%	0.7%	2.4%	13%	11%
Relative standard deviation of all results (%)	1.1%	2.8%	3.8%	2.6%	8.7%	8.1%

Table 10
Comparisons of spectra

Laboratory	Code name	Peak-to-valley ratio of Compton peak	Secondary to primary Compton ratio
1	EGS-NRC-MP	2.14	0.11
1bis	PENELOPE 3	2.02	0.09
2	LD1	1.7	0.08
3	PENELOPE 3	2.25	0.13
3b	MCNPX 2.5d3	2.25	0.11
4	GEANT 3	2.32	0.10
5	LD2	2.75	No secondary peak
6	MCNP 4c2	2.43	0.12
7	LD3	2.50	No secondary peak
8	LD4	2.0	0.11
8b	PENELOPE	2.17	0.12
9	LD5	2.65	0.09

gamma ray absorption probability calculation to the uncertainty budget of the ^{54}Mn standardization can be lower than 1%. Presumably, the uncertainty on the detection efficiency of the electron capture branch without gamma ray absorption is higher.

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