Simulation of Radioactivity in Liquid Scintillator

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We studied the usage of the radioactivity generator in G4dyb and simulated the radioactivity in liquid scintillator. To get correct simulation results, the time structure of the G4dyb output must be analyzed, besides the multiplier 4 for Thorium and 9 for Uranium. The requirements to the radioactivity of $GdCl_3{\cdot}6H_2O$ is set to be < 5 ppb for ^{238}U, < 10 ppb for ^{232}Th, and < 0.5 ppb for ^{40}K, according to the simulation results.

1 The Radioactivity Generator

^{40}K, ^{238}U, and ^{232}Th are discussed in the note.

^{40}K has two decay branches, 89.3% for β decay (end point = 1.31 MeV) and 10.7% for γ decay (1.46 MeV). The ^{40}K generator in the Daya Bay code repository does not include the β decay. However the β decay can not be neglected in the background simulation of liquid scintillator (LS). We include the β decay in the ^{40}K generator for this simulation. The energy spectrum of β is taken from LBNL Isotopes Project [1].

The Uranium and Thorium radioactivity generator in the Daya Bay code repository is a fortran package from Andreas Piepke. To be specific, let's call it **AP generator**. The generator is also studied in DYB-doc-441 by Jianglai Liu and Chris Mauger. The generator includes all isotopes in U and Th series and all α, β, and γs. As explained in the code, it is assumed that the decay series is in secular equilibrium. Members of the series with short life time are created together with a correlation time. All correlated events are stored as a single generator event. However, these *short* lift times are normally long, from seconds to days. These correlated events are actually non-correlated in our detector. Therefore, time structure of the simulation output should be analyzed to get each single trigger.

The cascade decay of ^{238}U includes 14 cascades. The 14 decays are divided into 9 branches in AP generator, as shown in Fig. 1. Each branch is a generator event. We have assumed the decay series is in secular equilibrium. Thus each branch is generated with equal probability. One Becquerel of ^{238}U corresponds to 9 events per second in AP generator. A multiplier 9 will be applied to get the single rate in the following simulation.

The cascade decay of ^{232}Th includes 11 radioactive isotopes in 10 cascades. The 10 cascades are divided into 4 branches in AP generator, as shown in Fig. 2. As the Uranium

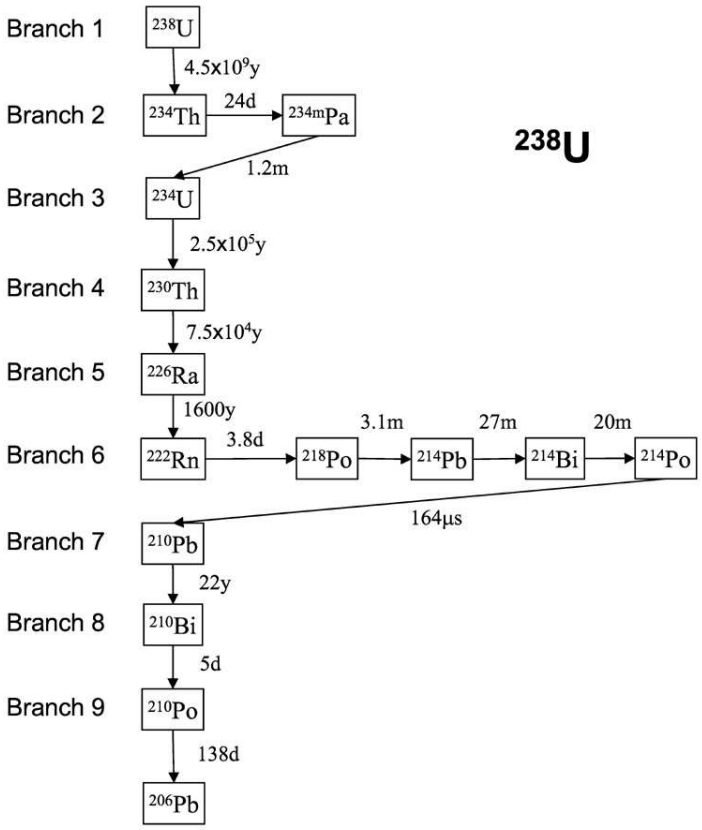

Figure 1: The decay chain of ^{238}U and branches in AP generator.

series, one Becquerel of ^{232}Th corresponds to 4 events per second in AP generator. A multiplier 4 will be applied to get the single rate in the following simulation.

The electronics of Daya Bay detector has a shaping time of around 300 nanoseconds. An event won't be triggered if it follows another trigger in 300 ns. In the analysis of simulation output, the photoelectrons (p.e.) are sorted by time at first. If two photoelectrons has time interval greater than 300 ns, they are divided into different sub-events. The photoelectrons are summed for each sub-events. If the total p.e. of a sub-event passes threshold, it will be triggered as a single. In principle, two or more cascade decays in a generator event could pile up and form one sub-event. But it has negligible chance to happen except the ^{212}Po $\rightarrow^{208}$ Pb decay in the Thorium series, which has a half-life of 299 ns. The second shortest half-life is the ^{214}Po $\rightarrow^{210}$ Pb in the Uranium series, which has a half-life of 164 μs.

2 Simulation of Radioactivity in Gd-LS

In the following, we assume the radioactivity of Gd-LS is 10^{-3} ppb, or 10^{-12}g/g, for ^{40}K,

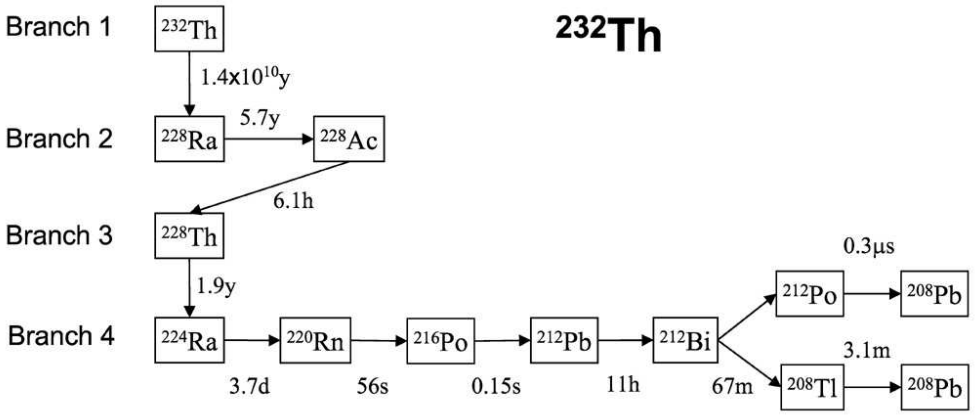

Figure 2: The decay chain of ^{232}Th and branches in AP generator.

^{238}U, and ^{232}Th each. Using the conversion relation

$$\begin{aligned} 1\,\text{ppb} \quad {}^{40}\text{K} &= 258.4\ \text{mBq/kg}\,, \\ 1\,\text{ppb} \quad {}^{238}\text{U} &= 12.4\ \text{mBq/kg}\,, \\ 1\,\text{ppb} \ {}^{232}\text{Th} &= 4.0\ \text{mBq/kg}\,, \end{aligned} \tag{1}$$

we get 5.2 Bq of ^{40}K, 0.25 Bq of ^{238}U, and 0.08 Bq of ^{232}Th for 20-ton Gd-LS.

10000 events are simulated using G4dyb for ^{40}K, ^{238}U and ^{232}Th each. They are generated uniformly in the Gd-LS volume of AD. As described above, the 10000 events include 10.7% 1.46 MeV gammas and 89.3% betas for ^{40}K. In the 10000 Thorium events, each of the 4 branches has 25% share. In the 10000 Uranium events, each of the 9 branches has 11.1% share.

To convert photoelectrons to visible energy, the 1.46 MeV gamma events of ^{40}K are selected for energy calibration. The gauss fit of the photoelectron spectrum is shown in Figure 3. We get 178 photoelectrons corresponding to 1.461 MeV. Assuming the detector response is linear, 1 MeV energy corresponds to 122 photoelectrons.

The energy spectra of ^{40}K, ^{238}U, and ^{232}Th are shown in Fig. 4, Fig. 5, and Fig. 6, respectively. If every cascade decay has more than 1 photoelectron in AD and there is no pile-up events, we should see 10000/9*14=15555 entries for U and 10000/4*10=25000 entries for Th.

Given an energy threshold, we define a ratio ϵ as

$$\epsilon = N_{\text{triggered}}/N_{\text{generated}}, \tag{2}$$

where $N_{\text{triggered}}$ is the number of sub-events above energy threshold and $N_{\text{generated}}$ is number of events, 10000 here. Note that ϵ is not the fraction of events that pass the threshold since there could be multiple sub-events passing the threshold in one generated event. The single

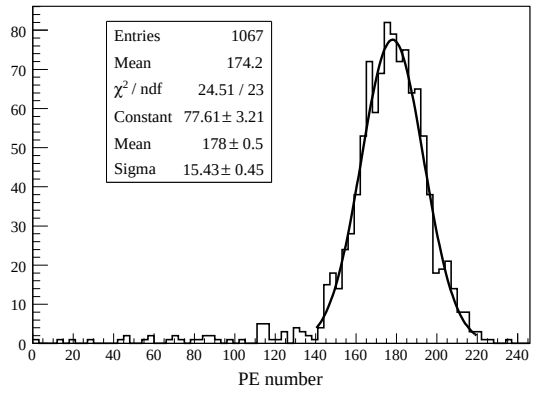

Figure 3: Gaussian fit of the p.e. spectrum of 1.46 MeV γ from ^{40}K.

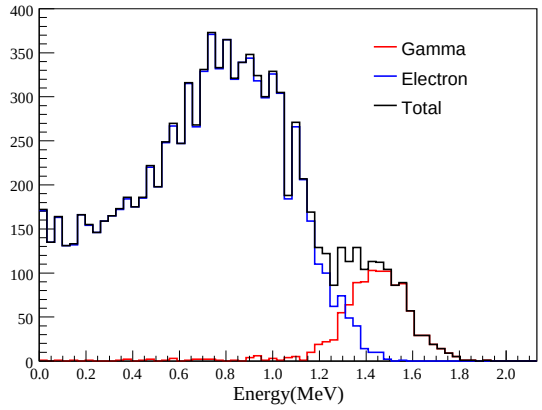

Figure 4: The energy spectrum of ^{40}K in Gd-LS.

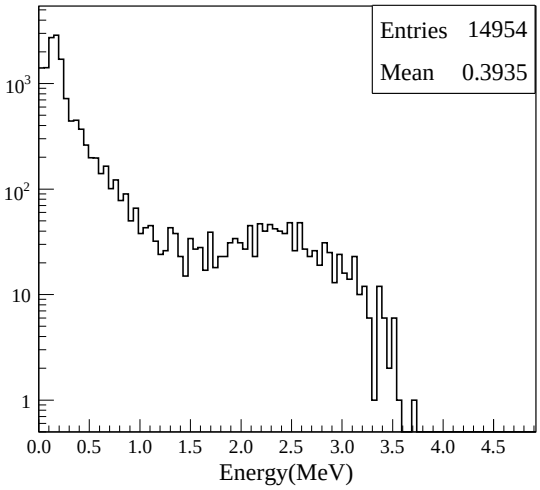

Figure 5: The energy spectrum of ^{238}U in Gd-LS.

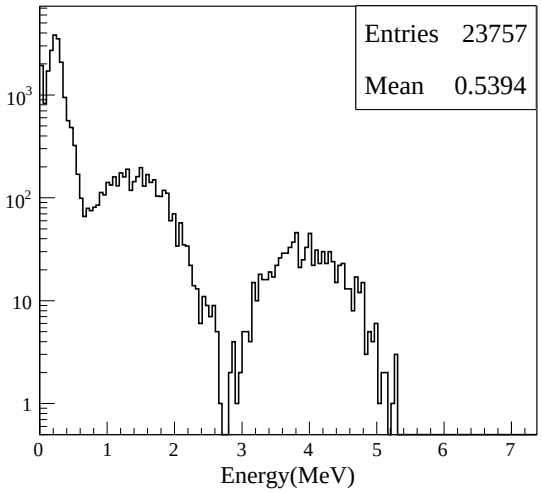

Figure 6: The energy spectrum of ^{232}Th in Gd-LS.

rate is

$$\text{Rate} = \epsilon \times R \times M, \tag{3}$$

where R is the radioactivity of 20 tons Gd-LS and the multiplier M is 4 for ^{232}Th and 9 for ^{238}U. The obtained single rates are listed in Table 1.

If we don't analyze the time structure of the simulation output, all decays in one branch will pile up in one event. As an example, the energy spectrum of ^{232}Th is shown in Fig. 7. There are a lot of high energy events, up to 6.8 MeV. Obviously the spectrum is incorrect. When calculating the single rate with energy threshold 1 MeV, we get 0.34 Hz for U and 0.15 Hz for Th, quite similar to the correct one. Comparing to the above sub-event analysis, the total entries is less but there are more high energy events. The resulting single rate happen

	1 MeV		0.5 MeV	
	ϵ	Rate (Hz)	ϵ	Rate (Hz)
10^{-3} ppb ^{40}K	27.9%	1.44	74.8%	3.87
10^{-3} ppb ^{238}U	13.8%	0.31	25.7%	0.57
10^{-3} ppb ^{232}Th	38.9%	0.12	50.2%	0.16

Table 1: The single rates of ^{40}K, ^{238}U, and ^{232}Th in 20 ton Gd-LS, with 1 MeV and 0.5 MeV threshold.

to be comparable.

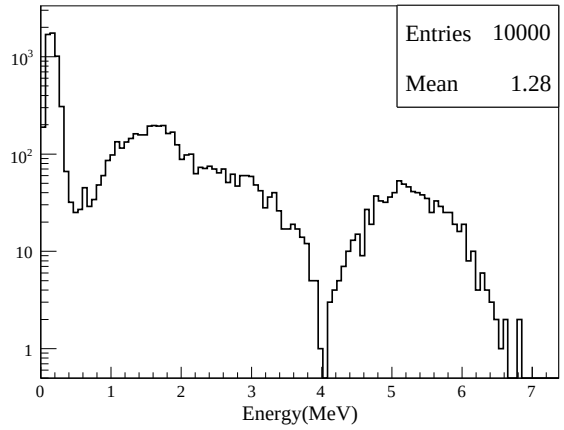

Figure 7: The energy spectrum of ^{232}Th with energies of all decays in one branch piled up.

2.1 Simulation of Radioactivity in γ-catcher

Similar to the simulation of radioactivity in Gd-LS, we did the simulation for normal liquid scintillator in γ-catcher. Again, 10000 events are simulated using G4dyb for ^{40}K, ^{238}U and ^{232}Th each. They are generated uniformly in γ-catcher.

The energy spectra of ^{40}K, ^{238}U and ^{232}Th in LS are shown in Fig. 8, 9 and 10. As expected, the simulation results are quite similar to the simulation for Gd-LS. The spectra shift to higher energy because for simplicity, we use the same p.e. to energy conversion as the Gd-LS simulation, while it is well known that more photoelectrons will be produced for events at larger radius. If the energy calibration can correct the vertex dependence very well, the energy spectra should shift to slightly lower end comparing to that in Gd-LS, because some γs will escape from LS. The energy smearing due to γ escape is observed in Fig. 10, where the valley at 3 MeV is not as sharp as that for Gd-LS.

The radioactivity of normal liquid scintillator should be orders lower than that of Gd-LS because the dominant radioactive source is the Gadolinium. Here we assume the same

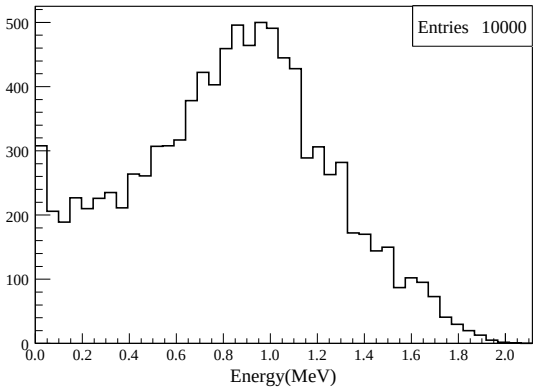

Figure 8: The energy spectrum of ^{40}K in γ-catcher.

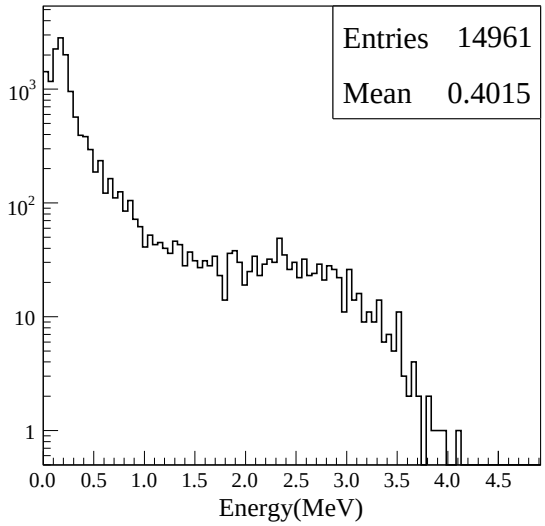

Figure 9: The energy spectrum of ^{238}U in γ-catcher.

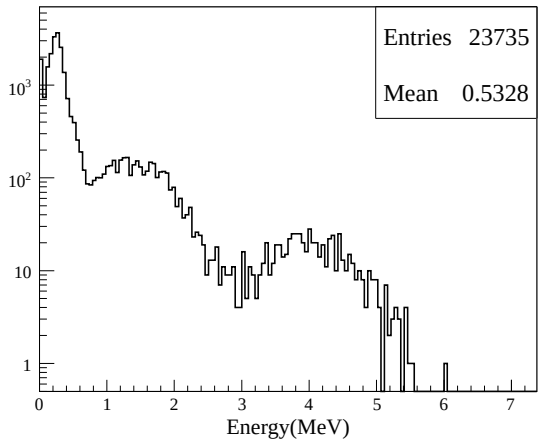

Figure 10: The energy spectrum of ^{232}Th in γ-catcher.

radioactivity as that of Gd-LS, i.e. 10^{-3} ppb for ^{40}K, ^{238}U, and ^{232}Th each. The total mass of normal liquid scintillator in γ-catcher is around 20 ton. The single rates are calculated as that of Gd-LS and listed in Table 2.

3 Comparison to DYB-doc-441

In DYB-doc-441 [2], the radioactivity in Gd-LS is studied using the AP generator, without detector simulation. α particles are ignored due to large quenching factor in liquid scintillator (10$\sim$20). True energy of β and γ is used to calculate the single rates in AD. Cut at 0.7 MeV,

	1 MeV		0.5 MeV	
	ϵ	Rate (Hz)	ϵ	Rate (Hz)
10^{-3} ppb ^{40}K	33.6%	1.73	75.8%	3.92
10^{-3} ppb ^{238}U	14.0%	0.31	26.4%	0.59
10^{-3} ppb ^{232}Th	36.7%	0.12	51.4%	0.16

Table 2: The single rates of ^{40}K, ^{238}U and ^{232}Th in γ-catcher, with 1 MeV and 0.5 MeV threshold.

10^{-3} ppb ^{40}K, ^{238}U, and ^{232}Th contribute 5.3 Hz, 0.43 Hz, and 0.14 Hz to the AD single rate, respectively. We included the detector response, studied the event pile-up, and the pile-up of α contributions to the β and γ energy using G4dyb. For example, the energy smearing could move more events to higher energy because the radioactivity events peak at low energy. The 9 MeV α from ^{212}Po $\rightarrow^{208}$ Pb could pile up to the β from ^{212}Bi $\rightarrow^{212}$ Po of end point energy 2.25 MeV. Our simulation shows that these effects are not significant, resulting in comparable single rates in two studies.

4 Requirements to Gadolinium radioactivity

The raw material of $GdCl_3$ is measured by Caltech and NUU for samples procured by IHEP and BNL. The radioactivities of ^{238}U and ^{232}Th are found to be from several hundreds ppb to 1.9 ppm [3]. Without purification, the gadolinium will contribute $\sim$ 500 Hz single rate in AD. According to the simulation, we can set the requirements to the purification.

The raw material is $GdCl_3{\cdot}6H_2O$. 1 ppb U and Th radioactivity in $GdCl_3{\cdot}6H_2O$ corresponds to 2.36×10^{-3} ppb in Gd-LS with 0.1% Gd concentration. Suppose we require the contribution of Gd-LS to the AD single rate to be smaller than 10 Hz, we have

	Isotopes	Radioactivity requirements	Corresponding AD single rate
$GdCl_3{\cdot}6H_2O$	^{238}U	< 5 ppb	3.7 Hz
	^{232}Th	< 10 ppb	3.1 Hz
	^{40}K	< 0.5 ppb	1.7 Hz

Table 3: Radioactivity requirements to the purified $GdCl_3{\cdot}6H_2O$.

From Fig. 1 and Fig. 2, ^{238}U, ^{234}U, ^{230}Th, ^{226}Ra, ^{210}Pb, ^{232}Th, ^{228}Ra, and ^{228}Th have half-lives longer than one year. They should be removed from the $GdCl_3$. Other isotopes has short half-lives and will decay in days. There are relatively mature and effective chemical procedures to remove U, Th, and Ra. For other isotopes, most will disappear after a week. The exceptions include:

- ^{210}Pb has half-life 22.3 years and could be problematic. In the chain below it, the

^{210}Bi $\rightarrow^{210}$ Po has beta decay of end point energy 1.161 MeV, which will contribute some to the AD single rate;

- ^{210}Po has half-life 138 days but they emit only α of energy 5.4 MeV thus can not contribute to the single rate;
- In the Thorium series, ^{228}Ac has half-life 6.1 hours. It will decay to ^{228}Th and be accumulated there, corresponding to 0.036% of original radioactivity. For example, suppose the ^{232}Th is 2 ppm before purification. After removal of all U, Th, and Ra, the ^{228}Ac will result in radioactivity equivalent to 0.72 ppb ^{232}Th. If we really want to remove it, another pass of purification can be done after all ^{228}Ac decay to ^{228}Th. But most likely it is not necessary.

References

[1] http://ie.lbl.gov/toi/

[2] Jianglai Liu and Christopher Mauger, DYB-doc-441.

[3] Christopher Mauger, DYB-doc-1368; Chung-Hsiang Wang, DYB-doc-1393.