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HFE and Spherical Cryostats MC Study

J. P. Brodsky

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Jason Brodsky

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1 Introduction

The copper vessel containing the nEXO TPC is surrounded by a buffer of HFE, a liquid refrigerant with very low levels of radioactive element contamination. The HFE is contained within the cryostat's inner vessel, which is in turn inside the outer vessel. While some HFE may be necessary for stable cooling of nEXO, it is possible that using substantially more than necessary for thermal reasons will help reduce backgrounds originating in the cryostats.

Using a larger amount of HFE is accomplished by making the cryostat vessels larger. By itself, increasing the cryostat size somewhat increases the background rate, as the thickness of the cryostat wall must increase at larger sizes. However, the additional space inside the cryostat will be filled with HFE which can absorb gamma rays headed for the TPC. As a result, increasing the HFE reduces the number of backgrounds reaching the TPC.

The aim of this study was to determine the relationship between HFE thickness and background rate. Ultimately, this work should support choosing a cryostat and HFE size that satisfies nEXO's background budget. I have attempted to account for every consequence of changing the cryostat size, although naturally this remains a work in progress until a final design is achieved. At the moment, the scope of the study includes only the spherical cryostat design.

This study concludes that increasing cryostat size reduces backgrounds, reaching neglible backgrounds originating from the cryostat at the largest sizes. It also shows that backgrounds originating from the inherent radioactivity of the HFE plateau quickly, so may be considered essentially fixed at any quantity of HFE.

2 Geometry

To understand the effect of cryostat size on backgrounds, six models were simulated. These six models are described in the table below.

Model	Inner Cryo Radius (cm)	IC Thickness (cm)	IC Mass (kg)	Outer Cryo Radius (cm)	OC Thickness (cm)	OC Mass (kg)	HFE Min. Thickness (cm)	HFE volume (m^3)
10 cm	102.6	0.45	112	157.6	1.05	620	10	2.7
30 cm	122.6	0.45	160	177.6	1.19	893	30	5.8
0	151	0.45	243	206	1.38	1393	58.4	12.7
Default	169	0.50	338	223	1.5	1774	76.4	18.5
1	181	0.54	416	236	1.59	2106	88.4	23.1
2	211	0.62	659	266	1.79	3012	118.4	32.2

The outer cryostat radius is 55 cm from the inner cryostat radius (except for the default model, at 54 cm separation). The HFE minimum thickness is calculated along the diagonal to the corner/rim of the TPC. Minimum Thickness $= ICR -$ Corner Radius, Corner Radius $= \sqrt{\text{TPC Vessel Radius}^2 + \text{TPC Vessel Half-Height}^2} = \sqrt{65.66^2 + 65.3^2} = 92.6\,\text{cm}$.

Wall thicknesses are for carbon fiber. LLNL engineer Allen House provided the formula wall thickness $= k \cdot$ radius, where $k = \frac{P}{2\sigma}$, $P = 0.079\,\text{MPa}$, $\sigma = 13.30\,\text{MPa}$ for the inner cryostat. The stress limit σ is probably greatly underestimated—it represents a safety factor of ~50 or more. The minimum thickenss is fixed at 0.45 cm to accomodate handling—Allen isn't ruling out thinner, but doesn't have the experience to rule it OK yet.

For the outer cryostat, the buckling concern under pressure makes the calculation more complicated. Allen calculated the best thickness with a FEA model with a target buckling load factor of 13.5 (considered extremely safe). The OC radius range 2130 - 2330 mmis well fit by the formula thickness [mm] $= 0.0068 \cdot$ radius [mm] $- 0.194$. It appears extrapolating this formula outside that range slightly overestimates the required thickness, resulting in a more conservative background estimation. These thickness requirements do assume a top hatch, but do not consider the possibility we will need more feedthroughs later which would increase the total cryostat mass.

Other relevant parameters, as simulated:

HFE Density (1 bar Xe boiling point)	1.77 g/cm^3	
HFE Density (room temperature)	1.4 g/cm^3	
Carbon Fiber Density	1.88 g/cm^3	

Andreas reports that the EXO-200 HFE was considered to have a density of 1.8 g/cm^3.

2.1 Stainless Steel Variant

Carbon fiber is nominally stronger, but due to the potential for buckling along its weaker axis, a carbon fiber outer cryostat must be somewhat thicker than the otherwise weaker stainless steel outer cryostat option. For the inner cryostat, Allen suggested using the same thicknesses for stainless and carbon fiber. Since stainless is weaker, the safety factor for this stainless inner cryostat is somewhat smaller, but still high enough, and all handling concerns should be fine.

Despite being no thicker than the carbon fiber option, stainless is substantially more dense, so the cryostat masses are higher.

Model	Inner Cryo Radius (cm)	IC Thickness (cm)	IC Mass (kg)	Outer Cryo Radius (cm)	OC Thickness (cm)	OC Mass (kg)
10 cm	102.6	0.45	466	157.6	0.64	1561
30 cm	122.6	0.45	665	177.6	0.72	2230
0	151	0.45	1009	206	0.83	3475
Default	169	0.50	1404	223	0.90	4405
1	181	0.54	1725	236	0.95	5218
2	211	0.62	2732	266	1.1	7465

SS Density	7.8 g/cm^3	

2.2 Inner Cryostat Liner

If the inner cryostat is made of carbon fiber, it will need a liner to ensure compatibility with the HFE. There are specialty plastics that would work for this purpose (cold-compatible), or we could use titanium. Allen's estimate is that we'll need a 1 mm thick liner.

Model	Inner Cryo Radius (cm)	Liner Volume (cm^3)	Titanium Mass (kg)	Plastic Mass
10 cm	102.6	13215	59.5	18.5
30 cm	122.6	18873	84.9	26.4
0	151	28634	128.9	40.1
Default	169	35870	161.4	50.2
1	181	41146	185.2	57.6
2	211	55920	251.6	78.3

3 Activity

Activies are reported with a calculated upper limit when a measurement and error are available. When only the upper limit is provided by the screening, only that is reported. For this U.L.-only measurements, calculations of total background rate assume a measurement of 0 activity and an error calculated to match the reported upper limit.

The upper limit is calculated by: $\text{Max}(A, 0) + 1.645 \cdot \sigma_A$, where the 1.645 constant is set by the desire to reach a 90% confidence level and the "flip-flop" consideration necessary when disallowing negative activity measurements from lowering the upper limit.

3.1 Carbon Fiber

Isotope	Activity (Bq/kg)	Error (Bq/kg)	90% U.L. (Bq/kg)	
Th232	1.1E-4	5.6E-4	1.3E-3	
U238	-4.0E-4	4.2E-4	6.9E-4	
Co60	1.5E-4	2.0E-4	4.8E-4	
K40	1.6E-2	6.2E-3	2.65E-2	
Cs137	-1.9E-4	4.2E-4	6.9E-4	

Screening ID R-0017.1.2

Note large relative errors. These large errors essentially drive the whole result.

Andreas points out that the priorities for screening are driven not just by which materials have large errors but also which materials have the largest contribution to the total background rate.

3.2 HFE

Isotope	Activity (Bq/kg)	Error (Bq/kg)	90% U.L. (Bq/kg)	
Th232	6.0E-08	3.7E-8	1.2E-7	
U238	1.9E-07	1.2E-7	3.9E-7	
K40	4.8E-06	2.9E-6	9.7E-6	

Screening JINST 7 P05010 (2012)

3.3 Stainless Steel

Isotope	Activity (Bq/kg)	Error (Bq/kg)	90% U.L. (Bq/kg)	
Th232			8.0E-4	
U238			6.0E-4	
Co60	1.68E-2	2.4E-3	1.74E-2	
K40	1.6E-2	6.2E-3	1.8E-3	

Screening R-020.1.1. This is the screening provided by Gerda

3.4 Titanium

Candidate for liners

Isotope	Activity (Bq/kg)	Error (Bq/kg)	90% U.L. (Bq/kg)	
Th232	2.8E-4	3E-5	3.3E-4	
U238			1.6E-3	
Co60			2E-5	
K40			5.4E-4	

There is a reasonable amount of scandium-46 (2 mBq/kg), but that does not have any radiation in the ROI.

4 Simulation Methods

To date, I have simulated 1E9 events per isotope per location per model. 1E10 event simulations are currently processing, as I have concluded that 1E9 event simulations leave us in a regime where we are less comfortable setting correct statistical upper limits.

I used the nEXO-MC version current as of 2015-11-25.

5 Background Definition

A simulated event is a background if it is a single-sited event with energy in the 1% FWHM and located in the inner 3 tons of liquid xenon.

5.1 Energy cut

The deposited energy must fall in the region of interest surrounding the double beta decay Q-value. The ROI is the full width half maximum around the Q-value, assuming a 1% energy resolution at the Q-value. That works out to the range 2428 - 2488 keV.

5.2 Single-Sited

Only single-sited events are considered to be backgrounds. Simulated events are clustered by an algorithm that groups together the energy depositions recorded by GEANT4. Any depositions within a certain small distance from each other are combined into a single cluster. An event is called single-sited if only one such cluster exists with energy above some (small) threshold. Notably, this technique does not incorporate any smearing, aliasing, or any other limitations of the real detector.

5.3 Position Cut

The hit efficiencies in section 6.1 are reported for the inner 3 tons of liquid xenon. This 3-ton region is defined according to the "old" shape, based on the standoff distance reference set to mimic older analysis. Re-analysis with an updated reference may change the results somewhat.

5.4 Decay Chains

When simulating the decay chains of ^{238}U and ^{232}Th, "one simulated event" is actual a simulation of one decay of each isotope in the chain. For simulation simplicity, isotopes unlikely to produce backgrounds in the xenon (e.g., alpha emitters) are not simulated.

As a result of this behavior, it is theoretically possible for one event to produce multiple backgrounds. However, the low efficiency of background production in general means that seeing hit efficiencies above 1 is never going to happen.

^{238}U-chain isotopes: ^{234}Pa, ^{226}Ra, ^{214}Pb, ^{214}Bi, ^{210}Tl

^{232}Th-chain isotopes: ^{228}Ac, ^{224}Ra, ^{212}Pb, ^{212}Bi, ^{208}Tl

6 Results

6.1 Hit Efficiencies

If B backgrounds are measured in N simulated events, the hit efficiency is estimated to be $\frac{B}{N}$. The error is estimated to be $\frac{\sqrt{B}}{N}$, except when $B = 0$ in which case the error is estimated to be $\frac{1}{N}$.

The 90% confidence upper limit of the hit effiency is defined using an inverse beta function: $\text{Beta}^{-1}(90\%; B+1, N-B+1)$. I assume this is the proper result for a Feldman-Cousins interval, but hopefully we end up explaining in more depth in another technical note.

6.1.1 10 cm

Co-60 was not simulated for this model.

Component	Chain	SS Hit Efficiency	SS Hit Error	SS Hit Efficiency Upper Limit	
HFE	Th	2.73E-06	5.23E-08	2.80E-06	
	U	2.83E-06	5.32E-08	2.90E-06	
IC	Th	1.01E-06	3.19E-08	1.06E-06	
	U	5.50E-07	2.35E-08	5.81E-07	
	Co				
OC	Th	3.54E-07	1.89E-08	3.80E-07	
	U	1.82E-07	1.35E-08	2.01E-07	
	Co				

6.1.2 30 cm

Component	Chain	SS Hit Efficiency	SS Hit Error	SS Hit Efficiency Upper Limit	
HFE	Th	1.56E-06	3.96E-08	1.62E-06	
	U	1.46E-06	3.83E-08	1.51E-06	
IC	Th	2.50E-07	1.58E-08	2.71E-07	
	U	7.10E-08	8.49E-09	8.31E-08	
	Co	0.00E+00	1.00E-09	2.30E-09	
OC	Th	1.11E-07	1.06E-08	1.25E-07	
	U	4.10E-08	6.48E-09	5.05E-08	
	Co	0.00E+00	1.00E-09	2.30E-09	

6.1.3 Model 0

Component	Chain	SS Hit Efficiency	SS Hit Error	SS Hit Efficiency Upper Limit	
HFE	Th	7.83E-07	2.80E-08	8.20E-07	
	U	7.04E-07	2.66E-08	7.39E-07	
IC	Th	3.16E-08	5.71E-09	4.01E-08	
	U	7.00E-09	2.83E-09	1.18E-08	
	Co	0.00E+00	1.00E-09	2.30E-09	
OC	Th	1.76E-08	4.31E-09	2.43E-08	
	U	0.00E+00	1.00E-09	2.30E-09	
	Co	0.00E+00	1.00E-09	2.30E-09	

6.1.4 Default Model

Component	Chain	SS Hit Efficiency	SS Hit Error	SS Hit Efficiency Upper Limit	
HFE	Th	5.36E-07	2.32E-08	5.66E-07	
	U	4.82E-07	2.20E-08	5.11E-07	
IC	Th	1.11E-08	3.48E-09	1.68E-08	
	U	2.00E-09	1.73E-09	5.32E-09	
	Co	0.00E+00	1.00E-09	2.30E-09	
OC	Th	4.67E-09	2.38E-09	8.86E-09	
	U	0.00E+00	1.00E-09	2.30E-09	
	Co	0.00E+00	1.00E-09	2.30E-09	

6.1.5 Model 1

Component	Chain	SS Hit Efficiency	SS Hit Error	SS Hit Efficiency Upper Limit	
HFE	Th	4.19E-07	2.05E-08	4.47E-07	
	U	3.83E-07	1.96E-08	4.09E-07	
IC	Th	4.31E-09	2.30E-09	8.40E-09	
	U	1.00E-09	1.41E-09	3.89E-09	
	Co	0.00E+00	1.00E-09	2.30E-09	
OC	Th	2.52E-09	1.88E-09	6.03E-09	
	U	0.00E+00	1.00E-09	2.30E-09	
	Co	0.00E+00	1.00E-09	2.30E-09	

6.1.6 Model 2

Component	Chain	SS Hit Efficiency	SS Hit Error	SS Hit Efficiency Upper Limit	
HFE	Th	3.09E-07	1.76E-08	3.32E-07	
	U	2.82E-07	1.68E-08	3.05E-07	
IC	Th	0.00E+00	1.00E-09	2.30E-09	
	U	0.00E+00	1.00E-09	2.30E-09	
	Co	0.00E+00	1.00E-09	2.30E-09	
OC	Th	3.59E-10	1.17E-09	2.90E-09	
	U	0.00E+00	1.00E-09	2.30E-09	
	Co	0.00E+00	1.00E-09	2.30E-09	

6.2 Background Rate Upper Limits

Here I report the central value, error, and 90% upper confidence limit for backgrounds. The error and upper limit are calculated using the current, "spreadsheet" method. The spreadsheet method is known to not correctly meet the 90% confidence target in some regimes, so I also report the U.L. calculated with the "algorithm" method that I developed to remedy some of the issues with the spreadsheet method.

All numbers reported are in backgrounds/year. They follow the definition of a background in section 5.

6.2.1 Model 0 cm

Component	Chain	Central Value	"Spreadsheet" Error	"Spreadsheet" 90% Conf. U.L.		
HFE	Th	1.56E-06	3.96E-08	1.62E-06		
	U	1.46E-06	3.83E-08	1.51E-06		
	Total					
IC	Th	2.50E-07	1.58E-08	2.71E-07		
	U	7.10E-08	8.49E-09	8.31E-08		
	Co	0.00E+00	1.00E-09	2.30E-09		
	Total					
Liner	Th					
	U					
	Co					
OC	Th	1.11E-07	1.06E-08	1.25E-07		
	U	4.10E-08	6.48E-09	5.05E-08		
	Co	0.00E+00	1.00E-09	2.30E-09		

7 Discussion

7.1 Bismuth-214

^{214}Bi may enter the HFE through the recirculation process. ^{238}U in the pipes (etc.) will decay into ^{226}Rn, which will diffuse into the HFE. In cold pipes, the diffusion rate is neglible, and so most radon will decay before making it into the HFE. However, the diffusion is significant at room temperature. Radon will quickly (time scale of days) decay down to ^{210}Pb, going through the decay of ^{214}Bi in the process. ^{214}Bi is the only isotope in that chain with a decay close to or above the ROI.

It's beyond the scope of this study (for the time being) to estimate an activity of radon diffusion into the HFE. Doing so will require a clearer picture of the surface area exposed to HFE and the temperature of those surfaces. A popular rule of thumb is that you can expect 1 radon atom per day per square meter of room temperature surface.

Existing simulations of the ^{238}U chaing show the hit efficiency for the specific isotope ^{214}Bi. It turns out that for the default model of the ^{238}U isotopes studied, *only* ^{214}Bi produces backgrounds in the 1% FWHM ROI. All other isotopes in the chain presumably do not produce backgrounds in the ROI at a signficant enough efficiency to survive the great filter of having to penetrate the TPC vessel and buffer xenon.

As a result, the quoted HFE ^{238}U hit efficiencies in section 6.1 can be used for radon-diffusion backgrounds as well as the inherent ^{238}U content of the HFE. That means that in the default model there will be one background for every ~2e6 radon atoms that diffuse into the HFE. Larger models tolerate more radon diffusion because the same amount of radon(/daughters) will be spread over more HFE, including HFE further from the TPC.

7.2 HFE Gamma Attenuation

HFE Composition	$C_3F_7OCH_3$	
Attenuation Coefficient	3.88E−2 cm^2/g	
HFE Density (1 bar Xe boiling point)	1.77 g/cm^3	
Attenuation Length	14.56 cm	

However, surprisingly the simulation results do not show a 14.56 cm decay constant. Instead, the decay constant is approximately 19 cm. My best explaination for this at the moment is perhaps a substantial fraction of the backgrounds are higher-energy γs that scatter down to the ROI energy. 4 MeV γs would have an absorption length of ~19 cm.

Explanations ruled out:

- The HFE density is correct in the simulation code.
- Using the minimum HFE thickness as the x-coordinate does not throw off the slope. If I replace the minimum HFE thickness with the true effective average thickness[1], it does not change the absoprtion length in the data.
- The effect of other shielding (Xe or otherwise) does not change the slope of the data.
- Any fixed-size components (e.g. flanges) would work in the other direction.

8 Auspices

LLNL-TR-703361

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[1] Averaging in log space