^{42}Ar Background in nEXO

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Abstract. The next-generation Enriched Xenon Observatory (nEXO) is a planned experiment utilizing 5 tonnes of isotopically-enriched liquid xenon (LXe) and a time projection chamber (TPC) to search for neutrinoless double beta decay of ^{136}Xe. The large, monolithic design of the nEXO TPC provides excellent shielding from the dominant background source - γ rays that originate from external materials. With an exceptionally clean central region of the TPC, we need to consider and quantify backgrounds that have previously been considered to be small relative to backgrounds from aforementioned γ rays or not considered at all. A case in the latter category is ^{42}Ar contamination in LXe. We will present the quantitative study of this ^{42}Ar background for nEXO.

INTRODUCTION

The next-generation Enriched Xenon Observatory (nEXO) experiment intends to search for neutrinoless double beta ($0\nu\beta\beta$) decay of ^{136}Xe. The central part of the nEXO detector is a time projection chamber (TPC) filled with liquid xenon (LXe) that is enriched to 90% in the nuclide of interest, ^{136}Xe. Five tonnes of LXe are to be used in the nEXO detector. The Q value for ^{136}Xe double-β decay, $Q_{\beta\beta}$, is 2458 keV [1, 2].

The different categories of background in nEXO are intrinsic radioactivity, steady-state ^{222}Rn in LXe, and exposure-based backgrounds, see Fig. 1 [3]. In the intrinsic radioactivity category, a new component was added in Ref. [3] compared to previous estimates: ^{42}Ar present in LXe. The focus of this presentation is the study of the aforementioned background component. The relevancy of this background for the nEXO experiment, the study of this background, and its contribution to the overall background budget will be discussed.

The number of single-site background events in the inner two tonnes of nEXO, in the energy interval $Q_{\beta\beta}\pm$FWHM/2 (2428-2488 keV), for one year of data taking is estimated at 0.5. Given the small expected background count, it is imperative to consider backgrounds that might be second or even third order. This consideration is especially crucial in the case of a background that resides in the very central region of the nEXO TPC such as the ^{42}Ar present in LXe.

RELEVANCE AND STUDY OF ^{42}Ar BACKGROUND FOR nEXO

Xenon is produced as a by-product of oxygen removal from air. The natural xenon thus obtained is then enriched to the xenon nuclide that is of interest (^{136}Xe) using centrifugal separation methods. The presence of argon in air implies that ^{136}Xe is produced with trace amounts of argon contained in it. This noble gas radioactivity is a concern to nEXO experiment. The argon isotopes that are relevant to the $0\nu\beta\beta$ search in nEXO are those that by themselves or via their daughters are long-lived enough to survive from procurement of xenon to the start of operations underground and have energy deposits that overlap with the FWHM energy window that is relevant to the nEXO experiment. Among argon isotopes, only ^{42}Ar qualifies for aforementioned conditions. The relevance of ^{42}Ar to the nEXO experiment can be seen from its decay chain,

$$^{42}_{18}\text{Ar} \xrightarrow[T_{1/2}\,=\,32.9\text{ y}]{100\%\ \beta^-} {}^{42}_{19}\text{K} \xrightarrow[T_{1/2}\,=\,12.4\text{ h}]{100\%\ \beta^-} {}^{42}_{20}\text{Ca (stable)}.$$

The end-point energy of the ^{42}Ar β-decay is at 599 keV [4] and therefore, by itself, ^{42}Ar is not a background for $0\nu\beta\beta$ search in nEXO. ^{42}K undergoes β-decay to ^{42}Ca with an end-point energy of 3525 keV [4]. A γ-ray with energy of 2424.3 keV (unresolved with the FWHM energy window) is coincident for 0.02% of the ^{42}K β-decays [4]. This coincident γ-ray has potential to be a background event for β-decays happening farther from the central region of the TPC. Thus, the decay of ^{42}K is a relevant source of background for nEXO.

To estimate the ^{42}K background for nEXO, we need to know the ^{42}Ar content in enriched xenon. Then, we use nEXO detector design information to determine the background rate from ^{42}K decays. Among the ^{42}K born in the nEXO detector, some fraction are ionic and migrate to biased surfaces. We model the distribution of ^{42}K in the detector

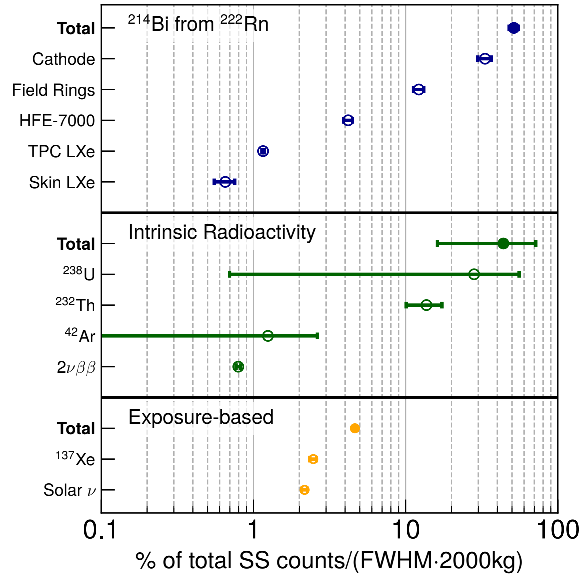

FIGURE 1. Single-site-like fractional background contributions with energy within $Q_{\beta\beta} \pm$ FWHM/2 and in the inner 2000 kg of nEXO detector [3].

and do simulation studies. The xenon is continually circulated and purified. The purification process can eliminate some of the ^{42}K from xenon. We model the circulation rate and the effect of the purifier to remove ^{42}K atoms from xenon. All these aforementioned steps are presented in the following sections to determine the background count from ^{42}K decays in the nEXO detector.

^{42}Ar CONTENT OF ENRICHED XENON

Many experiments have measured the relative content of ^{42}Ar in argon [5, 6, 7, 8, 9]. Since the natural abundance of ^{40}Ar isotope in argon is 99.6%, ^{40}Ar and natural argon are used interchangeably. These measurements were done from 1998 to 2019. The values reported in the literature are listed in Tab. I and range from 40 to 168 μBq/kg. These measurements provide an estimate of ^{42}Ar in natural argon.

TABLE I. Measurements of relative abundance of ^{42}Ar in ^{40}Ar.

Experiment	Year	Relative abundance of ^{42}Ar in ^{40}Ar	
		atoms/atom (10^{-21})	Specific activity (μBq/kg)
DBA [5]	1998	< 6 (90% C.L.)	< 60 (90% C.L.)
DBA [6]	2003	< 4.3 (90% C.L.)	< 43 (90% C.L.)
GERDA [8]	2014	$9.1^{+0.8}_{-2.0}$ to $16.8^{+2.2}_{-1.8}$	91^{+8}_{-20} to 168^{+22}_{-18}
DBA [7]	2016	$9.2^{+2.2}_{-4.6}$	92^{+22}_{-46}
DEAP [9]	2019	4.04 ± 0.59	40.4 ± 5.9

The EXO-200 collaboration measured the purity of their enriched xenon and reported the argon content to be $(7.6{\pm}1.8){\times}10^{-9}$ g/g [10]. Using atomic masses of ^{40}Ar and ^{136}Xe, the aforementioned measurement can be translated as 26 to 32 ^{40}Ar atoms among 10^9 enriched xenon atoms. The lower end of the range corresponds to the central value of measurement while the higher end corresponds to the central value plus 1σ uncertainty.

Besides one consideration, we can combine the aforementioned ^{42}Ar content in natural argon and the argon content in enriched xenon to obtain the ^{42}Ar content in enriched xenon. The consideration is that the centrifugal separation method is more efficient in removing lighter isotopes than heavier ones. Although ^{40}Ar is likely removed at a higher rate than ^{42}Ar, we are uncertain about their relative removal rates. Given that nEXO expects the heaviest xenon isotope (^{136}Xe) to be enriched to 90%, we assume a separation rate for ^{42}Ar relative to ^{40}Ar to be in the range of 1 to 9. Combining values for ^{42}Ar in natural argon (91-190 μBq/kg), argon content in enriched xenon (7.6 to 9.4 $\times 10^{-9}$ g/g), and the ease of removing ^{40}Ar relative to ^{42}Ar (a factor of 1 to 9), the specific activity of ^{42}Ar in enriched xenon is derived to be in the range of 0.7 to 16.1 pBq/kg. For a total LXe mass of 5000 kg in nEXO, the number of ^{42}Ar atoms is evaluated to be 5 to 119.

MODELING OF ^{42}K BACKGROUND IN nEXO

We begin with ^{42}Ar that is uniformly distributed in LXe and decays to ^{42}K. The differential equation for the rate of change of ^{42}K is

$$\frac{\mathrm{d}N_K(t)}{\mathrm{d}t} = \frac{N_A(t)}{\tau_A} - \frac{N_K(t)}{\tau_K} - N_K(t) \times (\frac{f}{V}) \times \varepsilon. \tag{1}$$

$N_K(t)$ is the number of ^{42}K atoms present in LXe at time t, $N_A(t)$ is the number of ^{42}Ar atoms present in LXe at time t, τ_A is the mean lifetime of ^{42}Ar, τ_K is the mean lifetime of ^{42}K, f/V is the fractional volume of xenon that encounters the purifier per unit time, and ε is efficiency of purifier to remove ^{42}K during recirculation. The first term is the creation of ^{42}K atoms from ^{42}Ar decays, the second term is the decay of ^{42}K, and the third term describes the interaction of ^{42}K with the purifier. The current representative xenon recirculation period is four days, f/V = 1/96 hour^{-1}. We do not have any estimates for ε. The derivation of number of ^{42}K decays in LXe is adapted from the mathematical treatment in Ref. [11]. The number of ^{42}K decays in 1 year is derived to be,

$$N_K^{1\text{ year}} = \frac{\mathscr{A}_A(0) \times M_{\mathrm{LXe}} \times \tau_A \times 0.0208}{1 + \tau_K \times \frac{f}{V} \times \varepsilon}, \tag{2}$$

where $\mathscr{A}_A(0)$ is the ^{42}Ar specific activity at $t = 0$, M_{LXe} is the mass of LXe contained in nEXO.

When ^{42}Ar decays, some fraction of the ^{42}K atoms is electrically neutral with the remainder being ionic. The fraction of ionic ^{42}K is not known via an independent measurement and is assumed to be equal to 0.764, the ionic fraction of ^{214}Bi from ^{214}Pb β-decay [12]. During the decay of ^{42}Ar, ^{42}K is uniformly produced in LXe. At production, ^{42}K atoms are distributed in active LXe and in inactive LXe per the relative masses of LXe in each region. In active LXe, neutral ^{42}K are uniformly distributed in LXe, while ionic ^{42}K drift to the cathode. Given the large difference in the half-life of ^{42}K and the drift time needed for ionic ^{42}K to drift to the cathode, a negligible fraction of ionic ^{42}K decay in active LXe. In other words, all ionic ^{42}K produced drift to the cathode and decay attached to the cathode.

Since the fraction of ionic ^{42}K is not known from direct observation, a conservative approach is to assume the fraction to be that which yields the largest background count. Since β-decays are highly localized, decays in active LXe are more probable to result in background events in the inner two tonnes than decays on the cathode. In this approach, the fraction of ions of ^{42}K is 0.0 and all ^{42}K atoms that are born in the active LXe decay uniformly in the active LXe.

We did simulations for ^{42}K in active LXe, inactive LXe and on the cathode. The energy spectrum of electrons from ^{42}K β-decays to the ground state of ^{42}Ca is "unique first-forbidden". We also confirmed that all γs coincident with the β-decay were properly simulated. Single-site (SS) and multi-site (MS) hit efficiencies for reconstructing ^{42}K disintegrations in the FWHM energy window and in the inner two tonnes of the TPC are listed in Tab. II. The SS efficiency for ^{42}K decays in inactive LXe and on the cathode can be ignored relative to the efficiency in the active region.

RESULTS

Based on simulation studies, we consider ^{42}K decays in active LXe to be the only relevant contributor. The number of background counts from ^{42}K decays in the inner two tonnes of nEXO for 1 year is shown in Fig. 2. In Fig. 2, we assume the ionic fraction of ^{42}K to be 0.76 and relative mass separation between ^{40}Ar and ^{42}Ar to be 9. Circulation

TABLE II. Efficiency for reconstructing ^{42}K disintegrations in FWHM energy window in the inner two tonnes. Numbers in parenthesis are statistical uncertainties expressed as a percentage.

nEXO part	Efficiency (10^{-3})	
	SS	MS
Active LXe	6.0 (0.4%)	2.2 (0.7%)
Cathode	7×10^{-5} (38%)	6.8×10^{-4} (12%)
Inactive LXe	6×10^{-5} (41%)	4.1×10^{-4} (16%)

time periods ranging from 1 to 6 days are considered while the efficiency of the purifier to remove ^{42}K atoms is shown in the x-axis. For the case of high recirculation time periods (much larger than τ_K) or the case of $\varepsilon = 0.0$, we expect 2.6×10^{-3} background events from ^{42}K in 1 year.

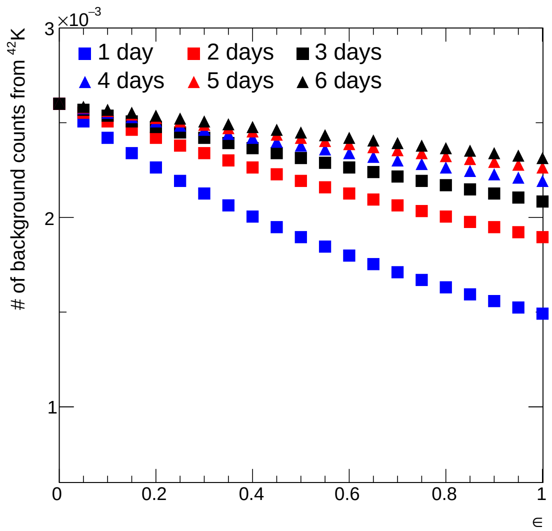

FIGURE 2. Number of background counts from ^{42}K in the inner two tonnes in 1 year for a range of xenon recirculation periods and as a function of the purifier efficiency to remove ^{42}K.

This study to evaluate the background contribution from ^{42}Ar present in LXe has a number of variable dependencies such as ε, f/V, the fraction of ionic ^{42}K, and ease for separation of ^{40}Ar relative to ^{42}Ar during the centrifugal process. We consider both extreme values of each dependency that would minimize and maximize the background. To that end, Tab. III lists background counts for every permutation of either extremes of each dependency. It is noted that the background count from ^{42}Ar present in LXe in the inner two tonnes in one year ranges from 7×10^{-5} to 1.1×10^{-2}.

SUMMARY

A central task of nEXO is to identify, study, and quantify backgrounds that are relevant to the experiment. We presented the background from ^{42}Ar in LXe. A similar analysis was done with the full EXO-200 dataset [11] and adapted to the nEXO experiment. Background from ^{42}Ar in the inner two tonnes of nEXO has been evaluated to be at most 2% of that from all other sources. At this scale, ^{42}Ar present in LXe will not significantly affect the sensitivity of nEXO experiment to observe $0\nu\beta\beta$ decay of ^{136}Xe.

TABLE III. Number of background counts from ^{42}K disintegrations in the energy interval $Q_{\beta\beta}\pm$FWHM/2 and in the inner two tonnes in one year for extreme values of various dependencies. The dependencies are ε, f/V , fraction of ionic ^{42}K ($f_{^{42}K^{+}}$), and ease for separation of ^{40}Ar relative to ^{42}Ar during the centrifugal process. The last column expresses background counts from ^{42}K as a fraction of the total nEXO background as evaluated in Ref. [3]. In the last row, the scenario with the lowest background count is rewritten using the lower end of range of ^{42}Ar specific activity in enriched xenon.

ε	f/V (day^{-1})	$f_{^{42}K^{+}}$	Relative mass separation ($\frac{^{40}\mathrm{Ar}}{^{42}\mathrm{Ar}}$)	$N_{\mathrm{bkg}}^{1\ \mathrm{year}}$	f_{BKG} (%)
0.0	1-4	0.76	9.0	2.6×10^{-3}	0.52
			1.0	2.9×10^{-4}	0.06
		0.0	9.0	1.1×10^{-2}	2.2
			1.0	1.22×10^{-3}	0.24
1.0	1	0.76	9.0	1.49×10^{-3}	0.30
			1.0	1.65×10^{-4}	0.03
		0.0	9.0	6.31×10^{-3}	1.26
			1.0	7×10^{-4}	0.14
	4	0.76	9.0	2.2×10^{-3}	0.44
			1.0	2.4×10^{-4}	0.05
		0.0	9.0	9.3×10^{-3}	1.86
			1.0	1.03×10^{-3}	0.21
1.0	1	0.76	1	7×10^{-5}	0.014

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