THEIA DBD White Paper

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1 Introduction

The THEIA search for neutrinoless double beta decay (NLDBD) aims for sensitivity to the non-degenerate normal hierarchy parameter space within the canonical framework of light Majorana neutrino exchange and three-neutrino mixing, at the level of $m_{\beta\beta} \sim 5$ meV. This is achieved through the loading of a very large mass of a NLDBD candidate isotope into an ultra-pure liquid scintillator target, together with coincidence and topological particle identification techniques.

2 Detector Configuration

Target Medium For the present studies, we consider a target that consists of pure LAB liquid scintillator loaded with the NLDBD isotope. This volume is contained within a nylon balloon, and the region of the detector outside is filled with water-based liquid scintillator (WbLS) with no isotope loading. With loading at 3% by mass, a 25 ton (50 ton) experiment corresponds to a 6.4 m (8 m) radius containment balloon.

The mass of LAB is obtained using a density of 0.86 g/cm^3, the optics are based on measurements by the SNO+ collaboration, and the backgrounds are based on measurements by SNO+, Borexino, and KamLAND-Zen.

Isotope Loading We consider possible NLDBD searches using two candidate isotopes: Te and Xe. In the case of Xe loading, xenon gas 89.5% enriched in ^{136}Xe is dissolved directly into the liquid scintillator, while Te loading is achieved via a novel technique developed for the SNO+ experiment and uses natural Te (34.1% ^{130}Te). The contamination associated with the materials used for Te loading are considered in the background assessment.

Additional NLDBD isotopes may be considered as long as they can be loaded into liquid scintillator. A staged approach is envisioned where an NLDBD observation in one isotope can be confirmed by removing it and deploying a second; the ability to switch isotopes is a key advantage of a liquid scintillator detector.

3 Backgrounds

The main sources of background near the NLDBD energy region of interest include:

Double Beta Decay This irreducible background is due to the $2\nu\beta\beta$ decays of ^{130}Te or ^{136}Xe. Due to the steeply-falling spectrum, the number of events falling in the ROI depends strongly on the energy resolution.

Cosmogenic Production These backgrounds are due to activation of nuclei by muons (during data taking) or protons and neutrons (during material production and handling at Earth's surface).

Solar Neutrinos The primary source is elastic scattering of ^{8}B solar neutrinos, though these events can potentially be reduced using the direction relative to the Sun. Another potential background is due to activation of the target material (Te or Xe) by the solar neutrinos, mainly ^{7}Be and ^{8}B neutrinos; this background is also dependent on the energy resolution.

Source	Target level	Expected events/y $r = 6.4$ m	$r = 8$ m
Balloon ^{10}C		250 – 800	500 – 1600
^{8}B neutrinos		1490	2950
^{130}I (Te target)		48 (9 from ^{8}B)	93 (18 from ^{8}B)
^{136}Cs (Xe target)		24 (3 from ^{8}B)	47 (6 from ^{8}B)
^{136}Cs (^{enr}Xe target)		245 (35 from ^{8}B)	478 (68 from ^{8}B)
$2\nu\beta\beta$ (Te target)		$3.8{\times}10^{7}$	$7.4{\times}10^{7}$
$2\nu\beta\beta$ (Xe target)		$3.6{\times}10^{6}$	$7.0{\times}10^{6}$
$2\nu\beta\beta$ (^{enr}Xe target)		$3.6{\times}10^{7}$	$7.1{\times}10^{7}$
Liquid scintillator	^{214}Bi: 10^{-17} g_U/g	3700	7300
	^{208}Tl: 10^{-17} g_{Th}/g	440	870
Nylon Vessel	^{214}Bi: $1.1< \times 10^{-12}$ g_U/g	$7.7{\times}10^{4}$	$1.2{\times}10^{5}$
	^{208}Tl: $1.6< \times 10^{-12}$ g_{Th}/g	$1.3{\times}10^{4}$	$2.1{\times}10^{4}$
PMTs	^{214}Bi: 10^{-6} g_U/PMT		
	^{208}Tl: 10^{-6} g_{Th}/PMT		

Table 1: Dominant background sources expected for the NLDBD search in Theia. It is assumed that the Te or Xe isotopes are directly loaded at a level of 3% in the LAB+PPO scintillator cocktail, for a total mass of 28.3 tonnes (6 m radius) or 55 tonnes (8 m radius).

Internal Contamination Decays from U- and Th-chain impurities present in the scintillator mixture. Due to the large Q value of the candidate NLDBD isotopes, the two important backgrounds are due to ^{214}Bi ($Q = 3.27$ MeV) and ^{208}Tl ($Q = 5$ MeV). The scintillator purity can be improved by purification techniques to levels better than 10^{-18}, as demonstrated by the Borexino experiment [1].

External Sources Decays from U and Th-chain impurities present in the balloon material, the external water-based liquid scintillator, the shielding water, and in the PMTs also contribute to the background. The two most important isotopes are ^{214}Bi and ^{208}Tl, as they decay by the emission of high energy ($E > 2$ MeV) γ rays that can travel long distances. These events can be reduced using a fiducial volume cut, though the balloon material remains the most important as it is closest to the target volume.

A summary of all the expected background events is given in Table 1.

3.1 Cosmogenic Backgrounds

The cosmogenically-induced background consists of nuclides produced by activation of the target material by neutrons, protons, and muons during production, handling, storage, and data-taking.

Long-lived, high Q value nuclides can be produced by neutron and proton activation mainly while the material is on the Earth's surface. The production in Xe and Te has been investigated by several authors [2–8]. Among the most important nuclides are ^{60}Co ($Q = 2.8$ MeV, $T_{1/2} = 5.27$ y) and ^{110m}Ag ($Q = 3.1$ MeV, $T_{1/2} = 250$ d). Mitigation of these background sources requires minimal exposure at sea level, a deep underground cool-down period, and chemical purification processes [9].

Neutron activation can also happen deep underground, while the experiment is running. Neutrons originate from the radioactivity and from muon-induced reactions in the rock. A water shield will provide a mitigation, as the majority of the neutrons will thermalize and stop before reaching the target material.

For the purpose of this paper, it is assumed that the material will have a minimum exposure time at sea level and will be stored underground long enough to allow all the potential cosmogenic-induced nuclides produced during the surface exposure to decay.

A different source of cosmogenic background is the muon activation of the material during the data-taking period. In particular a potential background is the production of ^{10}C ($Q = 3.65$ MeV, $T_{1/2} = 19.3$ s) by muon interaction with the carbon atoms of the liquid scintillator. The interaction is accompanied by the emission of two neutrons. ^{10}C decays via the emission of a positron of 1.87 MeV end-point energy, followed by the emission of a γ of 0.72 MeV total energy. A mitigation strategy for this background source consists of a three-fold coincidence technique as developed by Borexino and KamLAND [10, 11], making use of the muon trajectory, the 2.2 MeV γ emitted by the neutron capture, and the ^{10}C decay. Additionally, the γ may travel away from the positron stopping point several tens of centimeters. This event topology is different from the neutrinoless double-beta decay, in which the energy deposition is localized.

The event rate of muon induced ^{10}C decays can be estimated following Reference [12]. The muon flux expected at the Homestake 4850 level (4300 mwe) is 4.2×10^{-9} cm^{-2} s^{-1}, while the calculated average muon energy at the same depth is 293 GeV [13]. The LAB+PPO mixture has a ^{12}C density of 4.4×10^{31} atoms/kt. The following formula can be used to scale the density from the one measured in Borexino and KamLAND:

$$R_i = R_{data} \times \left(\frac{\langle E_\mu \rangle}{\langle E_{\mu,data} \rangle} \right)^{\alpha_{sim}} \times \frac{\Phi_\mu}{\Phi_{\mu,data}} \times \frac{n_{12C}}{n_{12C,data}} \tag{1}$$

where α_{sim} has been obtained from FLUKA/Geant4 simulation and is equal to 0.7621 for ^{10}C [14]. This results in about 300 events/kt/yr. Using Equation 10 in Reference [12] results in about 800 events/kt/yr. For this source of background a reduction of 92.5% is assumed based on what reached by Borexino [15]

3.2 Solar Neutrino Induced Background

^{8}B solar neutrino elastic scattering in the target material results in a background that is approximately flat across the NLDBD energy region of interest. The spectrum can be normalized using the total ^{8}B flux and best fit solar mixing parameters, as in Reference [16]. The expected rate is about 1200 events/yr/kt of target material.

Another source of background are the nuclides produced by charged current interaction of solar neutrinos with Te or Xe, in particular ^{130}Te and ^{136}Xe. A detailed study of the expected interaction rate is given in References [24, 25].

For ^{130}Te (34.08% natural abundance) a total of 33.7 SNU are expected, of which 6.1 SNU due to ^{8}B neutrinos and 20.9 SNU due to ^{7}Be neutrinos. The daughter isotope is ^{130}I in the 1^+ excited state. The excited states decay quickly to the first excited level, which decays with $T_{1/2} = 8.84$ min to the ground state via internal transition (branching ratio 84%, $E_\gamma = 40$ keV), or directly beta decays to ^{130}Xe with a Q value of 2.99 MeV (BR = 16%). The ground state beta decays with a Q calue of 2.95 MeV and a $T_{1/2} = 12.4$ h. Due to the long half life a tagging technique based on a delayed coincidence might have a small efficiency.

For ^{136}Xe (8.8573% natural abundance) a total of 68.8 SNU are expected, of which 9.8 SNU due to ^{8}B neutrinos and 46 SNU due to ^{7}Be neutrinos. The resulting isotope is ^{136}Cs in the 1^+ excited states. The excited states decay quickly to the ground state, which decays with $T_{1/2} = 13.16$ d via beta decay (branching ratio = 100%) with a Q value of 2.55 MeV. Again in this case, a tagging technique based on a delayed coincidence will have only a small effect on removing this source of background due to the long half life.

The expected rate of events is given in Table 1.

3.3 Double Beta Decay Backgrounds

The number of $2\nu\beta\beta$ decays for ^{130}Te is calculated using the half life measured by CUORE [17], $T_{1/2} = (8.2 \pm 0.2 \text{ (stat.)} \pm 0.6 \text{ (syst.)}) \times 10^{20}$ y. This results in a rate of events per year

$$R_{2\nu\beta\beta} = 1.33 \times 10^7 \times M \times f \tag{2}$$

where M is the mass inside the balloon in kt and f is the loading fraction of natural isotope, or 3.8×10^7 events/yr for the 3% loading and a 6.4 m radius balloon.

For ^{136}Xe, the half life measurement in [11, 18] is used, $T_{1/2} = (2.165 \pm 0.016 \text{ (stat.)} \pm 0.059 \text{ (syst.)}) \times 10^{21}$ y, for a rate of

$$R_{2\nu\beta\beta} = 1.26 \times 10^6 \times M \times f \tag{3}$$

or 3.6×10^6 events/y for the 3% loading and a 6.4 m radius balloon. In case a 89.5% enriched ^{136}Xe is used, the expected number of events is 3.6×10^7 events/yr within a 6.4 m radius balloon.

3.4 Scintillator Backgrounds

A high purity level required in the LAB+PPO cocktail used to fill the balloon can be obtained using various purification techniques, including liquid-liquid extraction, nano-filtration, steam stripping, and distillation. A level of 10^{-17} g/g in both U and Th has been demonstrated by the KamLAND [19] and the Borexino [20] experiments. More recently a purity level of better than 10^{-18} has been obtained for the Phase-II of Borexino [1]:

^{238}**U** $< 9.7 \times 10^{-19}$ g/g (95% CL from ^{214}Bi-Po)

^{232}**Th** $< 1.2 \times 10^{-18}$ g/g (95% CL from ^{212}Bi-Po)

In addition to chemical purification, delayed coincidence techniques can be used to reduce the number of ^{214}Bi decays falling in the ROI. ^{214}Bi ($T_{1/2} = 19.9$ min) beta decays to ^{214}Po with a Q value of 3.27 MeV in 99.979% of cases. Several experiments have shown that this decay can be tagged using the subsequent ^{214}Po alpha-decay ($T_{1/2} = 164.3\,\mu$s, $E_\alpha = 7.7$ MeV). A rejection of approximately 100% for ^{214}Bi decays falling the ROI has been shown as possible by the SNO+ experiment. In the remaining 0.021% of the cases ^{214}Bi alpha-decays to ^{210}Tl ($T_{1/2} = 1.3$ min), which beta decays to ^{210}Pb with a Q value of 5.5 MeV. An α–β delayed coincidence, can be applied in this case. However, due to the longer half-life of ^{210}Tl, the tagging technique is expected to be less efficient.

In the case of the Th chain, the most relevant isotope is ^{208}Tl ($T_{1/2} = 3.0$ min, 36% branching ratio), which beta decays to ^{208}Pb with a Q value of 5.0 MeV. An α–β delayed coincidence can help in the reduction of the number of isotopes falling in the ROI. However, also in this case, the longer half life will result in a smaller rejection factor compared to the ^{214}Bi case.

In addition to the LAB+PPO cocktail purity, any material associated with the NLDBD loading must be considered. SNO+ reports a target level after the 0.5% Te loading of around 10^{-15} and 10^{-16} g/g for the U-238 and the Th-232 chains, respectively. KamLAND-Zen [21] reports a purity of $(1.3 \pm 0.2) \times 10^{-16}$ g/g U and $(1.8 \pm 0.1) \times 10^{-15}$ g/g Th. Higher purity levels are achievable in principle by improving the target material purification technique, like the purity of the chemicals used to process the tellurium. A target purity of 10^{-17} g/g for both the U and Th chain has been assumed for the Theia experiment. This purity level require a reduction factor of 99.9% of the ^{214}Bi events in the ROI in order to reduce the internal background to a negligible level. Factor 10 worse purity would require a factor 10 better background reduction. The SNO+ experiment has shown that it is possible to reach a reduction of the ^{214}Bi background of more than 99.99% in the region of interest.

3.5 Balloon Backgrounds

Among the external background sources, the closest to the target volume are the ^{214}Bi and ^{208}Tl decays in the containment balloon. A typical balloon material is nylon, and the intrinsic purity levels can be found in [22]. The values, based on Borexino measurements, are 1.1 ppt and 1.6 ppt for U and Th, respectively. KamLAND-Zen has also measured the purity level of the nylon they used for their balloon. Results in Reference [23] give 2 ppt and 3 ppt for U and Th, respectively. The purity levels reached by Borexino are used as target levels for the Theia experiment. A nylon balloon with a thickness of about 45μm is assumed.

3.6 PMT Backgrounds

For the present discussion it is assumed that with a fiducial volume cut the background induced by the PMTs is negligible in the region of interest for Theia NLDBD studies.

4 Sensitivity Studies

4.1 Detector Modeling

In order to study sensitivity to NLDBD in Theia, the dominant backgrounds have been simulated using the Geant4-based RAT-PAC software package.[1] The detector is modeled as a cylinder with

[1] https://github.com/rat-pac/rat-pac

40 m radius and height, for a total mass of 50 kt, located in the Homestake mine at a depth of 4300 m.w.e. A PMT coverage of 5% has been used for the simulations, then rescaled according to the assumed light yield.

The model assumes a liquid scintillator contained in the balloon composed of LAB with 2 g/l PPO, while the volume outside the balloon is filled with a WbLS (10% LAB-PPO and 90% water). The optical properties of the LAB-PPO cocktail have been measured by the SNO+ collaboration. For the WbLS, the optical properties are obtained by weighting contributions of the LAB-PPO and water, and are consistent with benchtop measurements. A multi-component absorption and reemission model (i.e. separate absorption lengths and reemission probabilities for each of the cocktail component) are used in the simulation. Radioactive decays are simulated using the Decay0 code [26].

While event reconstruction algorithms remain under development, the reconstructed energy is approximated by assuming the Poisson limit of photon counting: the true deposited energy, accounting for quenching, is smeared out by a Gaussian resolution function corresponding to the light yield. As a baseline, an average light yield of 1200 PMT hits per deposited MeV is assumed (corresponding to about $3\%/\sqrt{(E)}$ energy resolution), except where noted.

4.2 Counting Analysis

To estimate the sensitivity, a single-bin counting analysis is employed. Since all backgrounds do not scale with isotope mass (e.g. solar neutrinos and external γ backgrounds), we use the Monte Carlo to evaluate the background expectation, establish a confidence region using the Feldman-Cousins frequentist approach, and derive an expected limit on the NLDBD half life:

$$\widehat{T}^{0\nu\beta\beta}_{1/2}(\alpha) = \frac{N \cdot \epsilon \cdot t \cdot \ln 2}{\mathrm{FC}(n = b, b; \alpha)} \tag{4}$$

where N is the number of atoms of active NLDBD isotope, ϵ is the efficiency, t the live time, and b the expected background. 'FC' refers to a Feldman-Cousins interval at confidence level α.

The NLDBD region of interest is defined by a a fiducial volume cut and energy window. The fiducial volume is 7 m for an 8 m radius balloon, which reduces backgrounds from the balloon material. The energy window is asymmetric about the Q value, from $-\sigma/2 \rightarrow 2\sigma$ of a Gaussian fit to the NLDBD signal peak; this maximizes signal acceptance ($\epsilon = 66.9\%$) while removing much of the steeply-falling two-neutrino DBD background spectrum.

To summarize the baseline background assumptions detailed above, we use a reduction factor for ^{10}C of 92.5%, ^{214}Bi 99.9%, balloon backgrounds 50%, and ^{8}B solar neutrinos 50%.

The expected event rates per year for a $^{\mathrm{nat}}$Te or $^{\mathrm{enr}}$Xe loaded Theia detector with an 8 m radius containment balloon are given in Table 2. In both cases, the loading is at the level of 3% by mass. In the Xe case, enrichment to 89.5% ^{136}Xe is used, while Te is in its natural form (34.1% ^{130}Te). Figure 1 shows the background spectra near the endpoint in the Te (Figure 1a) and Xe (Figure 1b) cases.

Following Equation 4, we obtain a sensitivity in terms of $\widehat{T}^{0\nu\beta\beta}_{1/2}$, and compute a corresponding limit on the effective Majorana neutrino mass $m_{\beta\beta}$ assuming a light neutrino exchange model with phase space factors from Kotila and Iachello [27] and using the IBM-2 matrix element [28] for definiteness. The 90% CL sensitivity is:

$$\mathbf{Te}: \; T^{0\nu\beta\beta}_{1/2} > 9.7 \times 10^{27} \text{ y}, \; m_{\beta\beta} < 6.7 \text{ meV}$$

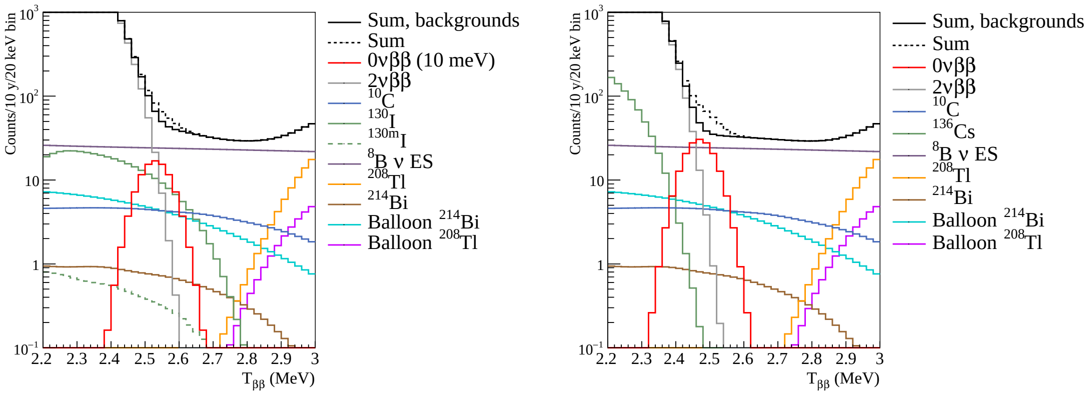
$$\mathbf{Xe}: \; T^{0\nu\beta\beta}_{1/2} > 2.6 \times 10^{28} \text{ y}, \; m_{\beta\beta} < 4.9 \text{ meV}$$

Energy Resolution The sensitivity is strongly dependent on the energy resolution, which in turn depends on the total detected light yield, since this sets of the level to which events in the steeply-falling $2\nu\beta\beta$ decay spectrum can migrate into the NLDBD energy ROI. Figure 2a shows the impact, holding other assumptions fixed.

Solar Neutrinos It is possible in principle to discriminate solar neutrino interactions from NLDBD signal, using Cherenkov light to determine the direction with respect to the Sun and possibly separate one- and two-ring topologies, on a statistical basis if not event-by-event. This is particularly important for Theia, where solar neutrinos are expected to be the largest background. Figure 2b shows the sensitivity scaling with solar neutrino event rejection.

Signal	Events/ROI·y Te Loading	^{enr}Xe Loading
$0\nu\beta\beta$ (10 meV)	65.4	116.4
$2\nu\beta\beta$	48.0	38.2
^{8}B Solar ES (50%)	138.5	138.4
^{10}C (92.5%)	24.6	25.4
^{130}I	48.3	—
^{130m}I	1.7	—
^{136}Cs	—	0.57
^{208}Tl	0.02	0.002
^{214}Bi (99.9%)	4.0	4.4
Balloon ^{214}Bi (50%)	24.0	27.4
Balloon ^{208}Tl (50%)	0.25	0.14
Total	289.5	234.5

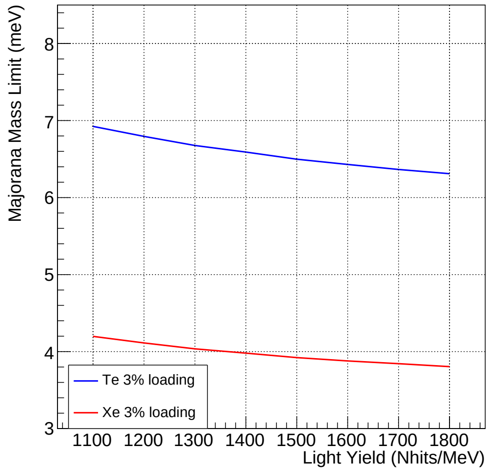
Table 2: Expected background counts per year in the ROI. In parenthesis is shown the reduction factor applied.



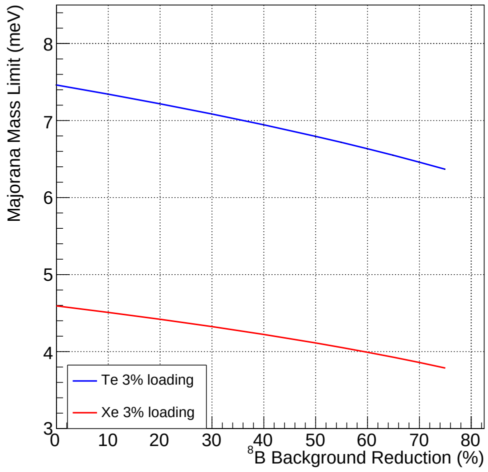
(a) Te loading

(b) Xe loading

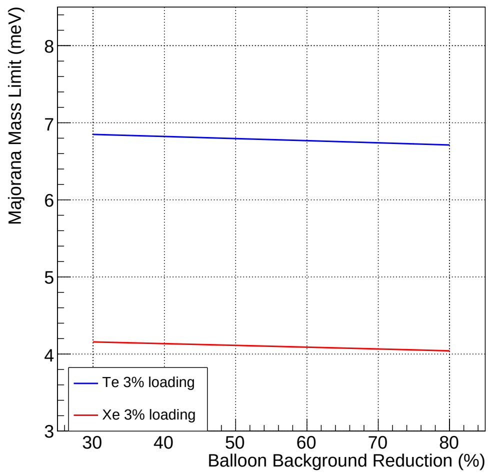
Figure 1: Energy spectra near the NLDBD endpoint for events within the 7 m fiducial volume.



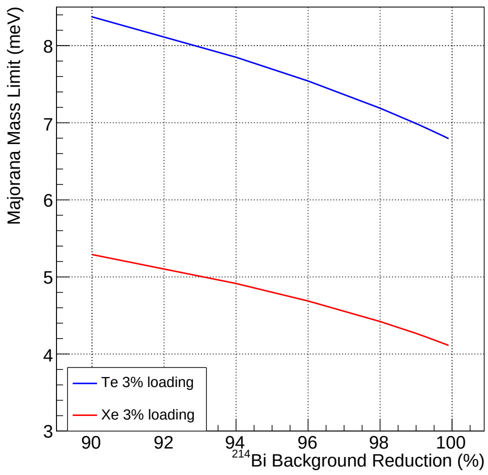
(a) Total detected light yield



(b) Reduction factor for ^{8}B solar neutrinos



(c) Reduction factor for external backgrounds



(d) Reduction factor for ^{214}Bi

Figure 2: Mass sensitivity as a function of key experimental parameters.

U/Th Chain Backgrounds The level of internal and external U and Th chain background reduction also depends on the power of timing and topology-based particle identification methods. Figures 2c and 2d show the sensitivity as a function of the external background and ^{214}Bi reduction factors, respectively, with other parameters fixed.

5 Conclusions

In summary, the Theia experiment can perform a very sensitive search for NLDBD, assuming a high level of Te or Xe loading and background levels near those demonstrated by previous experiments. We have performed a single-bin sensitivity analysis considering the dominant backgrounds for an experiment located at the 4850 foot level of Homestake, accounting for solar neutrino interactions, cosmogenic activation, and radioisotopic contamination of detector materials. We have studied the behavior of these backgrounds using a microphysical Monte Carlo simulation with a detector model including scintillator and WbLS optics. We find that for aggressive assumptions of radiopurity and background rejection, a Theia NLDBD search is capable of reaching sensitivity within the non-degenerate normal hierarchy parameter space.

6 Acknowledgements

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