Scintillation decay time and pulse shape discrimination in oxygenated and
ddeoxygenated solutions of linear alkylbenzene for the SNO+ experiment

H. M. O’Keeffe*, E. O’Sullivan, M. C. Chen

Department of Physics, Engineering Physics and Astronomy, Queen’s University, Kingston, Ontario, K7L 3N6, Canada

Abstract

The SNO+ liquid scintillator experiment is under construction in the SNOLAB facility in Canada. The success of this experiment relies upon accurate characterization of the liquid scintillator, linear alkylbenzene (LAB). In this paper, scintillation decay times for alpha and electron excitations in LAB with 2 g/L PPO are presented for both oxygenated and deoxygenated solutions. While deoxygenation is expected to improve pulse shape discrimination in liquid scintillators, it is not commonly demonstrated in the literature. This paper shows that for linear alkylbenzene, deoxygenation improves discrimination between electron and alpha excitations in the scintillator.

Keywords: Linear alkylbenzene, liquid scintillator, scintillator timing, pulse shape discrimination, SNO+

1. Introduction

The SNO+ experiment is currently under construction in the SNOLAB facility, located approximately 2 km underground in Sudbury, Ontario, Canada. The detector will consist of ~780 tonnes of linear alkylbenzene (LAB) liquid scintillator held in a 12 m diameter acrylic sphere and surrounded by 7000 tonnes of ultra pure light water shielding. An array of ~9500 photomultiplier tubes will detect scintillation light produced by particle interactions. Both the acrylic vessel and PMT array were inherited from the Sudbury Neutrino Observatory (SNO) experiment[1].

The SNO+ physics programme will include measurements of low energy solar neutrino fluxes and a search for neutrinoless double beta decay using neodymium[2]. Sensitivity to both requires precise energy and position reconstruction, for which an accurate characterization of the scintillator timing is needed. The scintillator decay time can be used to discriminate between alpha and electron events which occur in the scintillator, helping to exclude backgrounds and further improve sensitivity.

The focus of this paper is the measurement of the timing profile of liquid scintillator that will be used in the SNO+ experiment, namely linear alkylbenzene with 2 g/L 2,5-diphenyloxazole (PPO). Linear alkylbenzene was chosen because of its high flash point, low toxicity and acrylic compatibility. PPO will be added to the LAB at a concentration of 2 g/L as the primary fluor, emitting scintillation light across a wavelength region in which the SNO+ photomultiplier tubes are most efficient.

Measurements of scintillator decay times for electron and alpha excitations were made for oxygenated and deoxygenated samples of LAB with 2 g/L PPO. These measurements were made using the single photon sampling technique[3]. This method has been used to derive the decay times of many common liquid scintillators, including pseudocumene[4]. This paper will briefly discuss the theory of the single photon counting method and the experimental apparatus used in this work. Finally, results for each configuration of LAB will be presented and conclusions drawn.

*Corresponding author: okeeffe@owl.phy.queensu.ca
2. Scintillator timing profile

When an ionizing particle enters the scintillator, it can excite a linear alkylbenzene molecule which non-radiatively transfers this energy to a PPO molecule. Scintillation light is then emitted over a finite time period, via radiative de-excitation of the excited PPO molecule. The timing profile is a measure of the intensity of scintillation light as a function of time due to a single event. Timing profiles for organic scintillators usually consist of several exponential decay components. Radiative transitions to the ground state are permitted from singlet, but not triplet, excited states. The light produced by the singlet state de-excitation occurs quickly and is associated with the fastest component in the timing profile. When excitation to a triplet state occurs, a number of light producing de-excitation channels are available. For example, two triplet state molecules could collide, allowing simultaneous population of the singlet excited state and decay to the ground state. When compared with the singlet state de-excitation, such processes occur over a longer time period and are therefore associated with the longer timing profile components. The shape of the timing profile is related to the ionization density of the charged particle interacting with the scintillator. The relative contribution of singlet and triplet states to the timing profile depends on the ionization density of the particle. This results in differences in the shape of the scintillation light waveform which can be used to discriminate between particle types. Of particular importance for the SNO+ experiment is discrimination between alpha and electron events in the scintillator. Both solar neutrino and neutrinoless double beta decay events will produce electron-like signals in the detector. The ability to identify alpha events enables their rejection. Since alpha particles produce high ionization density, the proportion of the fast component relative to the slow component is reduced because of ionization quenching [3]. Conversely, due to their lower ionization density, the timing profile of electron events is dominated by the fast component.

3. Experimental measurement of the timing profile

The timing profile can be measured using the single photon sampling discussed in [3]. In this method, the light produced by a sample of scintillator is observed by two photomultiplier tubes (PMTs) connected to fast timing discriminators. The first PMT observes all events and provides a trigger for the electronics chain. The second PMT is covered by a mask containing a small hole in the centre, which allows single photons to be detected. The unmasked PMT provides a reference (start) time for each event. A finite time later, a single photon is detected by the masked PMT which defines the end of an event. The time difference between the start and stop of each event is recorded. By producing a histogram of these delayed coincidence events, accounting for the background and timing resolution, the timing profile of the scintillator can be obtained.

A schematic diagram of the apparatus used in this work is shown in Figure 1. A glass dish containing ~50 ml of LAB with 2 g/L PPO scintillator was optically coupled to a 5 cm diameter PMT (Electron Tubes Ltd 9266KB). The second PMT (Electron Tubes Ltd 9266KB) was covered with a mask containing a ~1 mm diameter hole. The signal from each PMT was connected to an independent channel of a fast timing discriminator (Phillips 715). The discriminator threshold for each PMT was set by using the discriminator signal to gate an MCA energy spectrum. For the masked PMT, the discriminator threshold was set such that the energy spectrum cut off just below the single photoelectron peak for all runs. For the unmasked PMT, the discriminator threshold was set such that a suitable energy threshold was selected, which was the same for alpha and electron runs. This ensured the zero offset of the timing spectrum was identical for all runs. The output from the unmasked PMT discriminator was connected to the start input of a time to amplitude converter (TAC) (ORTEC 566). The masked PMT discriminator channel was connected to the stop input of the TAC. A range of 500 ns was used for the TAC time window. The output of the TAC was connected to a PC running the Maestro multichannel analyzer (MCA) data acquisition software, which recorded the time difference for each event in terms of MCA channels.

Cesium-137 was used to obtain a sample of electrons via Compton scattering of the 662 keV gamma. The discriminator threshold was set to accept the full Compton edge. An americium-241 source was used to produce a sample of alpha events. This source was immersed in the scintillator and the discriminator threshold was set to exclude the 59 keV gamma, but include the full 5.48 and 5.44 MeV (quenched) alpha peaks.

Coincidences between the PMTs could be caused by non-scintillation events. To characterize this, complementary background runs were taken before and after each timing run. In a background run, the radioactive source remained in place and the hole in the mask was covered to prevent detection of photons from scintillation. The background spectrum was dominated by fast coincidences from cosmic ray interactions in...
the PMT glass and random coincidences between dark noise events. Each background run was time normalized and subtracted from its corresponding timing run.

4. Timing calibration and resolution

The timing resolution was measured by removing the PMT mask, which allowed scintillation light to be recorded by both PMTs simultaneously. This produced a Gaussian distribution of timings, with sigma equal to the timing resolution of the apparatus. Delays ranging from ~5 ns to ~100 ns were introduced between the discriminator and the stop channel of the TAC. This additional delay shifted the mean of the Gaussian by a given number of MCA channels and the timing calibration was obtained by applying a linear fit to this data. A timing resolution of $1.9 \pm 0.2$ ns was obtained by fitting a Gaussian distribution to this data along with a conversion factor of 16.98 ± 0.85 MCA bins per nanosecond.

5. Results

Measurements of scintillator decay times for electron and alpha excitations were made for oxygenated and deoxygenated samples of LAB+2g/L PPO. Deoxygenated samples were prepared by bubbling dry nitrogen through the sample for 20 minutes. To ensure the sample remained free of oxygen for the duration of the experimental run, the PMTs, scintillator and source were enclosed in an acrylic housing through which a slow flow of nitrogen was maintained. Timing profiles for the deoxygenated and oxygenated mixtures are shown in Figure 2.

The timing profiles shown in Figure 2 have been peak normalized to facilitate comparison between the two modes of excitation. The first portion of the curve is similar for all curves, but those for alpha excitations appear to fall off more slowly indicating, as expected, the presence of a long tail component.

To extract the timing components, a function consisting of three decaying exponentials which were individually convolved with a Gaussian was fitted to the background subtracted data. Fits with fewer exponentials returned a poorer chi squared per degree of freedom and those with more resulted in duplication of timing components. Therefore, three exponential terms were used in each fit. Each convolved exponential was multiplied by a scaling factor which represented the weighting of that component in the fit. The function fitted to the data was

$$\sum_{i=1}^{3} A_i \exp \left( \frac{x}{t_i} \right) \frac{0.25}{\sigma t_i^2} \sqrt{\frac{\pi}{4\sigma}} 1 + erf \left( \sqrt{\sigma \left( -x - \frac{0.5}{t_i} \right)} \right)$$

(1)

where $A_i$ is the scaling factor for each exponential component, $t_i$ is the timing component in MCA bins, $x$ is the MCA bin and $\sigma$ is the timing resolution (equivalent to 1.9 ns). The relative contributions of each component is given by

$$R_i = \frac{A_i t_i}{\sum_{i=1}^{3} A_i t_i}$$

(2)

where $R_i$ is the relative contribution for the $i$th component of the fit and $A_i$, $t_i$ were derived from (1). The TF1 function fitting class, found in the ROOT analysis
framework was used to perform the fit to the data. A cross check was made using the ROOFIT software also found in ROOT. Results from the TF1 fit are shown in Table 1.

Results for the timing components show significant differences between alpha and electron timing profiles for both the oxygenated and deoxygenated scintillators. Oxygen is responsible for quenching the longer lived decay processes. Deoxygenating the scintillator reduces the quenching and thus increases the relative amount of the longest timing component. It is clear that deoxygenation has a greater effect on the timing profile of alpha events. This enhances differences between the timing profiles of electron and alpha scintillation events, implying that pulse shape discrimination should be more effective in deoxygenated samples of linear alkylbenzene.

By defining a peak region in the timing distribution and comparing the integral of this region to the total integral, a peak to total ratio could be calculated. To assess the difference between the calculated ratios for alpha and electron events, 300 points were randomly sampled from each timing distribution, which is approximately equal to the number of photons produced by a 5 MeV alpha or 0.5 MeV electron. The ratio was calculated by dividing the number of counts in the peak region by the total counts. Looping over this method many times gave a Gaussian spread. Ratios for both oxygenated and deoxygenated scintillators are shown in Figure 3.

In oxygenated linear alkylbenzene, approximately 99% of alphas can be rejected whilst retaining $>99\%$ of electrons. In the case of deoxygenated linear alkyl-
benzene and for the same peak region, $\geq 99.9\%$ of alphas can be rejected whilst retaining $\geq 99.9\%$ of electron like signals. This proves that removing oxygen from the scintillator leads to improved particle identification and thus rejection of alphas. This is of particular importance in large scale liquid scintillator experiments such as SNO+.

6. Conclusions

This work has shown that the scintillator timing profile for linear alkylbenzene contains multiple decay components. The relative amounts and values of these components are sufficiently different for electron and alpha events, that separation and thus discrimination between particle types is possible. By directly comparing measurements of oxygenated and deoxygenated scintillator, it has been demonstrated that removal of oxygen from the scintillator leads to improved particle identification and separation of alpha and electron like events. While deoxygenating scintillator is widely expected to improve pulse shape discrimination, it is not commonly demonstrated in the literature. This work is the first to conclusively show this is the case for linear alkylbenzene, a scintillator which will be used in several large scale neutrino physics experiments, including SNO+.

7. Acknowledgements

The authors would like acknowledge financial support from the Natural Sciences and Engineering Research Council of Canada (NSERC).

References

[1] SNO Collaboration. Nucl. Instrum. Meth., A449:172, 2000.
[2] M.C. Chen. Nucl. Proc. Suppl., 145:65, 2005.
[3] L.M. Bollinger. Rev. Sci. Inst., 32:1044, 1961.
[4] G. Ranucci. Nucl. Instrum. Meth. A, 350:338, 1994.
[5] W. R. Leo. Techniques for Nuclear and Particle Physics Experiments. Springer-Verlag, 1987.