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Preliminary study of the inclusion of Water-based Liquid Scintillator in the WATCHMAN Detector

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Abstract

This note summarizes an effort to characterize the effects of adding water-based liquid scintillator to the WATCHMAN detector. A detector model was built in the Geant4 Monte Carlo toolkit, and the position reconstruction of positrons within the detector was compared with and without scintillator. This study highlights the need for further modeling studies and small-scale experimental studies before inclusion into a large-scale detector, as the benefits compared to the associated costs are unclear.

ACKNOWLEDGMENTS

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FIGURES

NOMENCLATURE

SNL	Sandia National Laboratories
PMT	Photo-Multiplier Tube
WATCHMAN	WATer Cherenkov Monitor of AntiNeutrinos
WbLS	Water-based Liquid Scintillator
WLS	Wave-Length Shifting

1. INTRODUCTION

For several years, researchers at both Brookhaven National Laboratory (lead by Minfang Yeh, [1]) and Sandia National Laboratories (P. Feng [2]) have been developing water-based liquid scintillators (WbLS) to improve the light output of water-based detectors. Without the addition of scintillator, which converts ionization energy into light, water-based detectors rely on the detection of Cerenkov light. Because Cerenkov produces much less light per unit energy deposited, water-based detectors have relatively poor energy and position resolution. This is usually mitigated by a combination of dense photo-detector coverage, reflective materials, and wavelength shifting (WLS) panels or chemicals to collect as much light as possible, taking care to preserve the directionality of the Cerenkov cone if the particular application requires it. In the case of WATCHMAN, directionality of the Cerenkov cone aids in the reconstruction of the position of the positron and neutron resulting from inverse beta decay within the volume both to fiducialize an inner region without optical separation and to require proximity in the positions of the positron and neutron. Both of these requirements reduce backgrounds significantly, and therefore this study focuses on the impact of WbLS on the position reconstruction in the WATCHMAN detector.

2. MONTE CARLO STUDIES OF POSITION RECONSTRUCTION

A Geant4 model of the nominal design of the WATCHMAN detector has been constructed in order to evaluate the optical response of the detector. The model includes all major components, including the correct layout of 5052 twelve-inch Hamamatsu photomultiplier tubes (PMTs) in the inner volume, the support structure, and the water volume doped with 0.1% gadolinium. For this study, the veto region is not instrumented with PMTs. The surface of the inner volume is modeled as a perfect optical absorber. Physical processes such as Rayleigh scattering, optical absorption, Fresnel reflection at the water/PMT surface, and Cerenkov radiation generation are included. Figure 1**Error! Reference source not found.** illustrates the detector model, and Figure 2 shows wavelength-dependent optical processes included in the base model without WbLS.

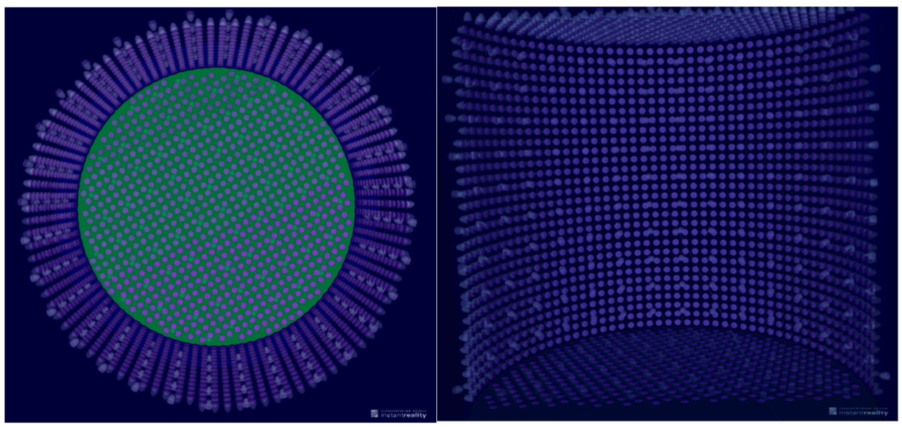

Figure 1: The Geant4 detector model from above (left) and the side (right). The model includes all major detector components, such as the correct placement of the 5052 PMTs in the inner volume.

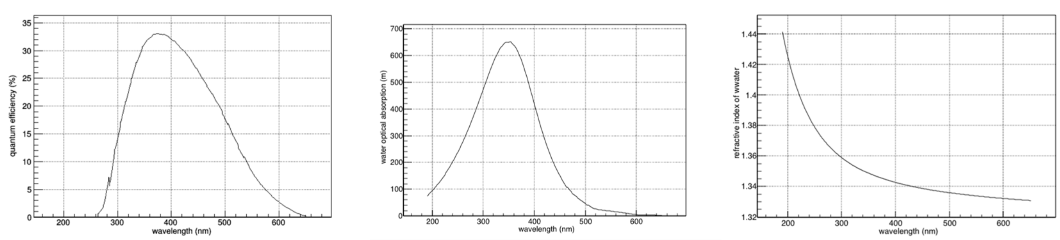

Figure 2: The wavelength-dependent optical processes included in the baseline model: the PMT quantum efficiency of the high-efficiency 12-inch Hamamatsu PMTs (left), the optical absorption of the water volume (taken from Super-K, assuming no degradation from the gadolinium, center), and the refractive index of the water (right).

In order to evaluate the impact of WbLS on the position reconstruction capabilities, the nominal performance of the detector without WbLS is first determined: the timing residuals of each PMT hit is minimized using the MINUIT software included in the ROOT [3] analysis toolkit:

$$\sum_{i=0}^{N}(t_i - t_0) - \frac{n}{c}|r_0 - r_i|.$$

The reconstructed interaction position, r_o, and time, t_0, are adjusted until the sum of all N PMT hit times minus the propagation time to each PMT is minimized. In the simulation, mono-energetic positrons are uniformly distributed throughout the inner volume of the detector. A basic trigger condition is applied, requiring that at least 16 PMTs have a signal greater than one photo-electron. The timing of the PMT hits are determined by the time of the first photon in the event to hit a particular PMT, and a Gaussian smearing is applied with a width of the expected PMT timing resolution of 1.37 ns. Individual photon hits are smeared by 40% to account for the PMT single photo-electron resolution, however no data acquisition modeling (i.e. electronics noise, digitization) aside from the trigger condition is applied. Due to the lack of realism in the detector response, the results here should be considered the best performance possible with respect to the timing resolution of the true WATCHMAN detector. Once detector response is included, the effects of the WbLS are likely to be worse than what is found in this work.

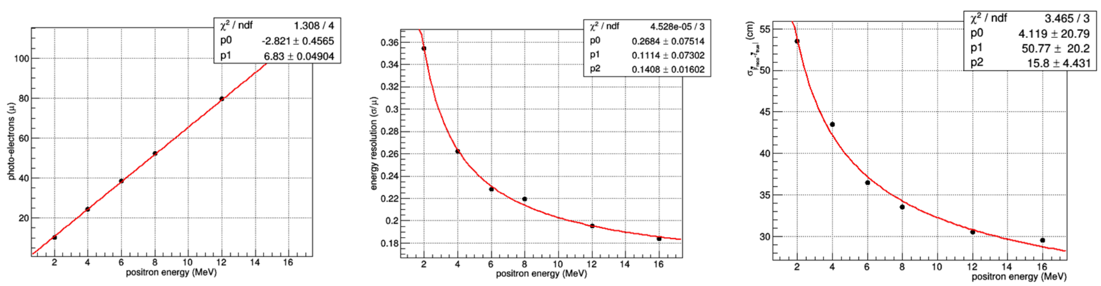

Figure 3: The number of photo-electrons measured as a function of incident positron energy (left), the energy resolution as a function of incident positron energy (center), and the one sigma position relative to the true position as a function of incident positron energy (right) with the nominal WATCHMAN detector design and no WbLS. The one-sigma position drops to 25 cm for energies greater than 16 MeV. For positrons resulting from reactor antineutrinos with an average energy closer to 3 MeV, the expected one-sigma position resolution is around 46 cm.

Figure 3 shows the results of the position and energy reconstruction for the nominal WATCHMAN detector with no WbLS included. The average number of detected photoelectrons per MeV of incident positron energy is 6.8, and the energy resolution (σ/μ) is ~30% at 3 MeV. The one-sigma reconstructed position is ~46 cm at 3 MeV.

Representative optical parameters for WbLS provided by P. Feng were then added to the Geant4 optical model. The typical cocktails used include three components: 99% of the composition is an organic solvent (which has WLS properties) and 1% of the composition is the primary fluorophore. In addition, very small amounts of another WLS compound are used in order to shift the scintillation light to an energy range visible to PMTs. Geant4 models scintillation and wavelength shifting properties, however only one of each process for a given particle type can be used by default. Therefore, in our study the scintillation emission is treated as the spectrum resulting from the fluorescence energy transfer to the WLS compound, a nearly 100% efficient process. An additional WLS process from the organic solvent is added, which has a ~17% quantum efficiency. This cut is applied in post processing for all optical photons resulting from the WLS process, as Geant4 does not currently handle WLS quantum efficiency. It should be noted that both the scintillation and WLS processes in Geant4 are isotropically emitted, and therefore will cause degradation of the Cerenkov cone.

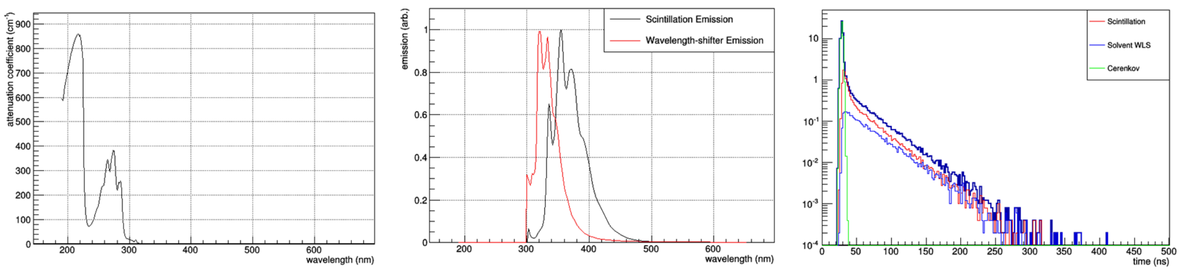

Figure 4: The Geant4 optical properties added to study the effects of WbLS: on the left is the attenuation co-efficient of the organic solvent, and in the center are the emission spectra of both the WLS-shifted scintillator (black) and the organic solvent emission (red). The pulse shape hitting the photo-multipliers (in a spherical detector with 100% photocathode coverage) is shown on the right, along with the contributions from each process. The Cerenkov component is very fast (green), whereas the scintillation (red) and solvent (red) nearly equally contribute to the slow tail of the pulse.

Figure 4 shows the optical properties included for the study of WbLS: the absorption of the organic solvent occurs primarily in the UV-blue wavelengths, and therefore will absorb the portion of the Cerenkov spectrum not usually visible by PMTs. The emission spectrum of the scintillator (black curve, on the right) is well matched to the quantum efficiency of the PMTs used in this study. M. Yeh's composition differs in the emission spectrum of the scintillator due to an additional secondary fluorophore, resulting in a final emission in the 385-423 nm range which is not as well matched to the PMT quantum efficiency used in this study. The organic solvent (red curve, on the right) will cause diffusion as the UV portion of the Cerenkov spectrum is absorbed and reemitted along the length of the particle track. The concern is that, while the scintillation is adding some additional light at the interaction location (with a yield of 100/MeV for this study, comparable to compositions of M. Yeh), the organic solvent is both causing light losses and adding a diffuse background. Finally, the timing of both the scintillation and WLS processes is not optimal: the scintillator compounds follow a 3-component exponential, with the fast component at nanosecond timescales, the middle component in the tens of nanoseconds, and slow component in the 100's of nanoseconds. Cerenkov radiation occurs in sub-nanosecond timescales, and adding these slow components will worsen the ability to reconstruct interaction positions. For this study, again due to Geant4's limitations, only the first two components are included at the ratio of 90% fast (3.5 ns) to 10% middle (35 ns). In reality, the fast component of the scintillation pulse is 90% of the total, the middle 7%, and the slow

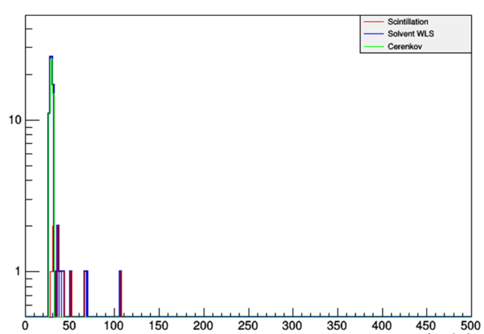

Figure 5: The resulting photon hits from a 4 single MeV positron at the center of a spherical detector with 100% photocathode coverage.

3%. For the solvent, the timing follows a bi-exponential function with a fast component (35 ns) comprising 96% of the total, and a slow component the remaining 4%. Only the fast component is included in this study. The slow (150 ns and 200 ns for the scintillator and solvent, respectively) components could add an additional diffuse uncorrelated background, however this effect is not explored here. Figure 4, right, shows the average arrival times of photons from 5k four MeV positrons at the center of a spherical detector with 100% photocathode coverage to obtain a representative pulse shape. Each optical process is shown individually, as well as the total pulse. The slow tail of the pulse contains nearly equal contributions of the solvent and slow scintillation component. Cerenkov light accounts for 76.5% of the total pulse shape, scintillation light 18%, and wavelength shifted light from the solvent 5.5%. Figure 5 shows the photon hits from a single 4 MeV positron in a spherical detector with 100% photocathode coverage: there are a total of 64 photons detected in this event.

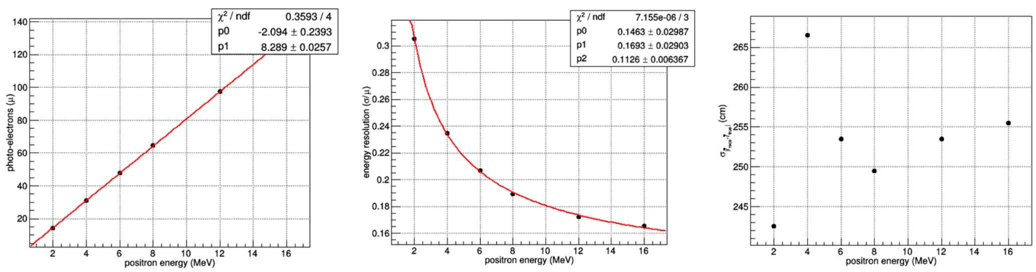

Figure 6: The number of photo-electrons measured as a function of incident positron energy (left), the energy resolution as a function of incident positron energy (center), and the one sigma position relative to the true position as a function of incident positron energy (right) with the nominal WATCHMAN detector design and WbLS included. The one-sigma position does not follow the standard expected function, and is around 250 cm at 3 MeV.

Figure 6 shows the same results as Figure 3, but with the WbLS processes included. The results indicate that, although there is additional light leading to an increase in energy resolution, the impact on the position resolution is large. The average number of photoelectrons has increased from ~6.8/MeV to ~8.3/MeV, leading to an energy resolution of 26% at 3 MeV compared to 30%, a small improvement considering the complication of its use (development of filtering methods, development of large volume production, and potential loss of position and timing resolution). Not surprisingly, using the same position reconstruction algorithm, the one-sigma resolution 46 cm to ~250 cm at 3 MeV. This position resolution is too poor to fiducialize the inner volume of the detector as desired: it is over 1.5x the shielding thickness intended for WATCHMAN (150 cm). There are possible improvements that could be made to the reconstruction algorithm, such as incorporating the expected pulse shape into the reconstruction algorithm, however it is not clear whether the previous position resolution can be regained.

3. CONCLUSIONS

These studies suggest that the benefits of WbLS should be taken as uncertain, and that further study is necessary to determine whether they can be realized. Additional work is currently being undertaken by a group of scientist for the Advanced Scintillator Detector Concept [4], lead by G. Gann at UC Berkeley. Better reconstruction algorithms, perhaps coupled with improved timing of photo-detectors, could help realize increased energy resolution and position reconstruction with the addition of WbLS. Further development into WbLS compounds could also be beneficial: increasing light yields, decreasing the slow component of the scintillator, or reducing the solvent re-emission could mitigate some of the concerns raised by this study. Research by P. Feng et al. has demonstrated increased light yields and reduced delayed emission through molecular design of the scintillator components, although these compositions are presently limited to water concentrations of less than 75% by volume. Work is ongoing to maintain these favorable scintillation attributes while increasing the water content, as required for sufficient optical transparency in large-scale applications such as WATCHMAN.

4. REFERENCES

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