Simulation study of optical degradation monitoring in the SNO+ experiment using an LED-based calibration system

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Abstract

Simulations of optical degradations of the liquid scintillator material in the SNO+ experiment has been performed, by reducing the absorption lengths of the scintillator material. An In-depth analysis of the simulated data was done, in order to link the physics within the detector to the signal detected by the detector. Based on this a set of section in space and time in the detector was defined to narrow down signal hits of certain types. A measure for the optical degradation in the scintillator material, the \textit{DegradationMeasure}, was defined, based on the various sections. Since this measure is based on detected signals it can be applied to actual calibration measurements by the AMELLIE calibration system in SNO+, in order to detect degradations to the optical properties of the liquid scintillator. The main results of the \textit{DegradationMeasure} for the different AMELLIE simulations are included in Table 7.2 and Table 7.3.
The contents of Chapter 4, Chapter 5, Chapter 6 and Chapter 7 is based entirely on my own work. All simulations referred to in the report has been performed by myself under the guidance of my supervisor, Lisa Falk.
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Chapter 1

Introduction

1.1 Neutrinoless double beta decay with SNO+

Within the Standard Model of particle physics, the neutrino has been the particle that has most challenged our current understanding of elementary particles. Experimental results obtained during the last 30 years, such as neutrino oscillations and neutrino masses, has contradicted the contemporary view of the neutrino. This has lead to an increase in the interest to study the neutrino in order to determine its properties and to look for new physics that might contradict the Standard Model.

The question of whether the neutrino is a Dirac fermion or a Majorana fermion, is the main topic of interest for some large scale particle physics experiments around the world. A profound consequence of the neutrino being a Majorana fermion, not a Direc fermion as the other fermions in the Standard Model, is that it allows for an extremely rare nuclear decay process known as neutrinoless double beta decay.

The SNO+ neutrino experiment in Sudbury, Canada, has the detection of the neutrinoless double beta decay process as its main research goal. It hopes to achieve this by studying the potential decay isotope, tellurium-130, dissolved in a liquid scintillator mix, that will be contained in a large detector volume located deep underground. A successful detection of neutrinoless double beta decay will be the rarest nuclear decay ever detected in an experiment. This impose strict requirements on the sensitivity of such an experiments, resulting in much work being done on detector design and calibration systems in order to ensure as precise measurements as possible.
1.2 Simulations of optical degradation in the scintillator mix

The work described by this report is relates to the calibration system designed for the SNO+ experiment. Specifically, the calibration subsystem designed to monitor the optical properties of the liquid scintillator mix in the SNO+ experiment. This is done by injection LED (light-emitting diode) light into the detector, in order to detect anomalies.

The purpose of the project described by this report is to attempt to predict how generic degradations of the liquid scintillator mix might be detected by the calibration system. Also, the project will attempt to determine how calibration measurements can be interpreted, and what measured anomalies might indicated about the optical properties of the liquid scintillator.

Studies of the optical degradation are performed using detailed Monte Carlo simulations of the optical calibration system for the SNO+ experiment. The studies includes an in-depth analysis of the detector simulations and the simulations of the physical processes within the detector. The in-depth knowledge about the simulations will be the foundation from which we base and justify our analysis of the simulated detector measurements.

1.3 Outline of the report

A presentation on the theoretical background of the project is given in Chapter 2 where the field of neutrino physics is described in the context of the Standard Model of particles physics. In addition, the theoretical phenomenon of neutrinoless double beta decay is described in Chapter 2 along with the present experimental status. Chapter 3 presents and describes the SNO+ experiment, as well as the optical calibration system that is the focus of this project.

In Chapter 4 the simulation framework that was used for the project is described, along with some basic output and analysis. This is in order to give an initial insight into the simulation features that will be the foundation of the further analysis. Next, Chapter 5 presents the way in which the simulation data is classified and visualised. This is done in order to obtain a way in which the most interesting and useful aspects of the simulated data can be isolated and viewed in a way that is relevant for the real life calibration measurements. Further, in Chapter 6 these classifications and visualisations are utilised in order to determine regions of interest that can be used for the real life calibration measurements. The defined regions of interests are then used in Chapter 7 to analyse a range of simulations. This analysis show how optical degradations on the scintillator
liquid can be detected with the optical calibration system. Finally, Chapter contains a conclusion of the project, where the project is summarised and the main results are presented.
Chapter 2

Theoretical background

2.1 Standard Model

Work within particle physics rely heavily on the Standard Model of particle physics. The Standard Model is a predictive theory of elementary particles and their interactions. It was formulated in the 1960’s and early 1970’s, combining the theory of electroweak interactions by Glashow [1], Weinberg [2] and Salam [3] and the theory of strong interactions by Fritzsch and Gell-Mann [4]. The Standard Model is based on extensive theoretical and experimental work going back to the beginning of the twentieth century. The latest major discovery predicted by the model was that of the Higgs boson in 2012, by the ATLAS [5] and CMS [6] collaborations at CERN.

The elementary particles described by the Standard Model can be separated into three groups of particles with different spin quantum number, which is an intrinsic property of elementary particles [7]. There are 12 elementary particles with spin quantum number $s = \frac{1}{2}$, also called spin-$\frac{1}{2}$ particles or fermions, which constitute the fundamental constituents of matter. These can further be separated into two groups: quarks and leptons.

There exists six quarks in the standard model, also called quark flavours, that differ by mass and electric charge. These are named: up, down, charm, strange, top and bottom. Quarks experience all four of the fundamental interactions: electromagnetism, the strong nuclear force, the weak nuclear force and gravity. The reason why quarks interact via the strong nuclear force is because they, in addition to electric charge, have another property called color charge. Quarks can be bound together by the strong force to form bound states that are called hadrons. For example, different combinations of three up and down quarks can form protons and neutrons, which are the particles that make up most of the mass of visible matter in the universe.
Then there are six lepton flavours: three charged leptons called electron, muon and tau, that differ by mass, and three neutral leptons called neutrinos. The three neutrinos are each related to one of the charged leptons through the weak nuclear force, hence their names: electron neutrino, muon neutrino and tau neutrino. None of the leptons experience the strong nuclear force, and carry no colour charge. All the leptons experience the weak nuclear force and only the charged leptons experience the electromagnetic force.

Next, there are four particles with spin quantum number $s = 1$, called gauge bosons or force carriers, that acts as mediators of the fundamental forces when exchanged between elementary particles. These are the photon, which mediates the electromagnetic force between charged particles; the gluon, which mediates the strong nuclear force between particles with colour charge, and the W and Z bosons, which mediates the weak nuclear force.

And then there is the Higgs boson [8, 9, 10], a particle with spin quantum number $s = 0$. The Higgs boson is a quantum excitation of the Higgs field, which explains why certain elementary particles have mass. Also, for each elementary particle in the Standard Model there exists an antiparticle with the same mass and opposite electric charge.

Mathematically, the Standard Model is an effective field theory, where the particles described above are represented by interacting quantum fields defined in space time.

The Standard Model of particle physics has been very successful in its predictions. One of the biggest successes has been the predictions of unknown particles that would later be experimentally discovered, sometimes between 20 or 30 years later. Notably one can mention the gluon, the W and Z bosons, the top quark and tau neutrino, but especially the Higgs boson, that was predicted about 50 years before its discovery. Also, the Standard Model has been very successful and consistent when applied to existing measurements in order to make further predictions for refined measurements. For example, measurements of the mass of the W boson have been very consistent with predictions based on radiative corrections [11, 12].

2.2 Beyond the Standard Model

Even though the Standard Model has been one of the most successful theories within physics and within the natural sciences, there is still a range of important physical phenomena that are either not explained by, included in or contradicting the Standard Model. The work of trying to explain these phenomena, and to modify the Standard Model in order to incorporate them, is called physics beyond the Standard Model (BSM). Physics
Beyond the Standard Model is an important focus of research within both theoretical and experimental particle physics, with the goal of getting closer to a “Theory of Everything”. In the following I will present some of the most substantial topics within BSM physics.

First, one of the biggest shortcomings of the Standard Model is that while it describes the three fundamental forces; electromagnetism and the strong and weak nuclear forces, it does not describe the gravitational force. Our present understanding of gravity is based on Einstein’s general theory of relativity [13], which is incompatible with quantum field theory. One attempt to include gravity into the relativistic quantum framework of the Standard Model is the proposal of the hypothetical massless and spin-2 boson called the graviton [14, 15]. Since the thirties, quantum gravity has been a been an active field within theoretical physics [16].

Secondly, the Standard Model of particle physics only describes 4.9% of the energy in the universe [17]. The rest of the energy is 26.8% dark matter and 68.3% dark energy. While dark energy is supposed to be related to the accelerated expansion of the universe and is mainly a topic within cosmology and astronomy, it is proposed that dark matter consists of unknown particles, currently not described by the Standard Model. A popular candidate for this are weakly interacting massive particles (WIMPs). WIMPs are defined as particles with large mass that only interacts with gravity and the weak nuclear force [18]. Some theoretical proposed dark matter candidates are the lightest supersymmetric particle (LSP), majorana fermions and sterile neutrinos.

Thirdly, the Standard Model has no clear explanation of the matter-antimatter asymmetry in the universe, the fact that there is no significant amount of antimatter in the universe compared to matter [19]. The popular explanation for this asymmetry is that in the very early universe ($\ll 10^{-11}$ s) there was a physical process called baryogenesis that produced the asymmetry. Such a process has to follow the Sakharov conditions [20]: baryonic number violation (1), C and CP violation (2) and a deviation from thermal equilibrium (3).

In attempts to solve some of the problems described above and other shortcomings of the Standard Model additional theories have been proposed, such as extra dimensions. Also, extensions to the Standard Model have been proposed, such as the Minimal Supersymmetric Standard Model (MSSM), that includes Supersymmetry (SUSY) [21].

In the next section I will present the field of neutrino physics, where experimental results have contradicted Standard Model assumptions and that could be a source of new physics beyond the Standard Model.
2.3 Neutrino Physics

In the early twentieth century, when a lot of research was focused on radioactivity, a very unexpected phenomenon occurred when studying beta decay (β-decay). According to nuclear physics at the time, when a carbon-14 decayed into a nitrogen-14 it would radiate a beta particle \((2.1)\), an electron, that would carry the energy \(Q\) roughly equal to the mass difference between carbon-14 and nitrogen-14.

\[
\text{C}^{14}_6 \rightarrow \text{N}^{14}_7 + e^- \tag{2.1}
\]

However, when measured, the energy of the electron had a continuous distribution instead of the energy \(Q\) \([22]\), as in Figure 2.1.

![Figure 2.1: Electron energy spectrum for beta decay of carbon-14. The red line marks the expected electron energy if only an electron were emitted. The blue line shows the observed electron energies. Figure by T2K Collaboration.](http://t2k-experiment.org/neutrinos/a-brief-history/betaspec/ (Accessed: 04.05.16))

The result baffled many physicists and it questioned whether conservation of energy applies at the atomic level. In order to save energy conservation, Wolfgang Pauli proposed in a letter in 1930\(^2\) a new particle, the neutrino, that was escaping detection with some of the energy, thus causing the beta spectrum. Further theoretical work based on Pauli’s neutrino idea was done, resulting in Enrico Fermi’s theory of beta decay in 1934 \([23]\), stating that a neutron inside the nucleus could decay into a proton, an electron and an antineutrino \((2.2)\).

\[
n \rightarrow p^+ + e^- + \bar{\nu}_e \tag{2.2}
\]

---
\(^1\)http://t2k-experiment.org/neutrinos/a-brief-history/betaspec/ (Accessed: 04.05.16)
\(^2\)http://microboone-docdb.fnal.gov/cgi-bin/RetrieveFile?docid=953;filename=pauli%20letter1930.pdf (Accessed: 04.05.16)
About 20 years later, in 1956, Clyde L. Cowan and Frederick Reines announced the first experimental evidence of the neutrino \cite{24}, an achievement for which Reines was awarded the Nobel Price in Physics in 1995 (Cowan passed away in 1974). In this experiment they detected the process called inverse beta decay:

\[
\bar{\nu}_e + p \rightarrow n + e^+, \tag{2.3}
\]

where the source of the electron antineutrinos was a nuclear reactor, and detection was done by detecting gamma rays from positron-electron annihilation and gamma rays from neutron absorption using cadmium-108.

It was shown by Raymond Davis that antineutrinos and neutrinos are distinguishable: A neutrino will convert chlorine-37 to argon-37 while an antineutrino will not \cite{25, 26}. The muon neutrino \((\nu_\mu)\) was detected by Lederman, Schwartz and Steinberger in 1962 \cite{27} (1988 Nobel Prize in Physics), and the tau neutrino \((\nu_\tau)\) was detected by the DONUT experiment at Fermilab in 2000 \cite{28}. The muon and tau neutrinos act in much the same way as the electron neutrino, except that when they interact, as in (2.2) and (2.3), the relevant electron or antielectron is replaced by a corresponding muon or tau lepton or antilepton respectively.

In the original Standard Model of particle physics it was assumed that the neutrinos were massless, that the lepton number \(L_i\) is conserved for each flavor \(i\), that neutrinos and antineutrinos are distinct, and that neutrinos are left-handed and antineutrinos right-handed\(^4\). While the rest of the Standard Model has to a large extent been verified by experiments, the Standard Model picture of the neutrino has been seriously challenged by experimental results in the last 30 years.

### 2.3.1 Neutrino Oscillations

A major upset to the Standard Model picture of the neutrino came as a solution to the solar neutrino problem. The first results of Raymond Davis’ and John Bahcall’s Homestake experiment, that detected neutrinos from the sun by the reaction

\[
\nu_e + \text{Cl}^{37}_{17} \rightarrow \text{Ar}^{37}_{18} + e^-, \tag{2.4}
\]

\(^2\)http://microboone-docdb.fnal.gov/cgi-bin/RetrieveFile?docid=953;filename=pauli%20letter1930.pdf (Accessed: 04.05.16)  
\(^3\)Lepton number = number of leptons - number of antileptons  
\(^4\)Left-handed: Spin antiparallel to momenta, Right-handed: Spin parallel to momenta
showed a deficit in measured neutrino flux compared to the calculated neutrino flux from the then current solar model [29]. Further solar neutrino experiments and improvements to the solar model continued to confirm this deficit. In addition to this, other experiments measuring atmospheric neutrinos saw a deficit of measured muon neutrinos compared to electron neutrinos, known as the atmospheric neutrino anomaly [30].

In the 80s and 90s a lot of work was done to try explain this strange phenomenon of the neutrino. One popular solution was that of neutrino oscillations, which Bruno Pontecorvo had presented in 1957 [31] and put forward as a solution to the solar neutrino problem in 1967 [32].

The theory of neutrino oscillations is based on the fact that the flavour eigenstates of the neutrinos ($\nu_e$, $\nu_\mu$, $\nu_\tau$) do not line up with the neutrino mass eigenstates ($\nu_1$, $\nu_2$, $\nu_3$). When a neutrino interacts weakly it does so in the form of one of the flavor eigenstates, which will be a superposition of the mass eigenstates. For a propagating neutrino, the quantum mechanical phases of the mass eigenstates advance differently because of the differences in their masses. Then when the propagating neutrino interacts again, it is a different superposition of the mass eigenstates, depending on the energy of the neutrino and the distance travelled. As a result, the probability of interacting as specific flavour eigenstate has changed. For example in the case of two neutrino flavors ($\nu_\alpha$, $\nu_\beta$) the probability of a neutrino of energy $E$ produced as a $\nu_\alpha$ to interact as a $\nu_\beta$ at a distance $L$ is given as

$$P_{\alpha \rightarrow \beta, \alpha \neq \beta} = \sin^2(2\theta) \sin^2 \left( \frac{1.27 \Delta m^2 L [eV^2][km]}{E[GeV]} \right),$$

where $\theta$ is the mixing angle between flavour and mass states and $\Delta m^2$ is the difference in squared masses of the mass states ($m_2^2 - m_1^2$). Experimental results by the Super-Kamiokande Observatory in 1998 [33] and the Sudbury Neutrino Observatory in 2001 [34, 35] gave convincing results of neutrino oscillations and were also awarded the 2015 Nobel Prize in Physics.

### 2.3.2 Neutrino masses

The phenomenon of neutrino oscillations also indicates, contrary to the Standard Model, that neutrinos have a non-zero mass and that the masses of the different mass eigenstates are different, since $\Delta m^2$ must be non-zero to allow neutrino oscillations. This leads us to the quest for determining the neutrino masses and discovering the origin of neutrino masses.

With neutrino oscillations experiments one can only measure the differences between...
squared masses, $\Delta_{ij}^2 = m_i^2 - m_j^2$ along with three mixing angles ($\theta_{12}$, $\theta_{23}$, $\theta_{13}$) and a CP-violating phase $\delta$. With regards to the squared mass differences, only two independent measures are needed, such as $\Delta m_2^2 = m_2^2 - m_1^2$ and $\Delta m^2 = m_3^2 - (m_1^2 + m_2^2)/2$. It is presently unknown whether the neutrino mass states are ordered such that $\Delta m_2^2 > 0$ ($m_1 < m_2 < m_3$) called normal hierarchy (NH) or $\Delta m_2^2 < 0$ ($m_3 < m_1 < m_2$) called inverted hierarchy (IH). A recent global fit (2013) of neutrino oscillation parameters is included in Table 2.1.

Table 2.1: Results of global 3$\nu$ oscillation analysis for normal and inverted hierarchy (2013). Table reproduced from [36].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>NH: Best fit 3σ</th>
<th>IH: Best fit 3σ</th>
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<tr>
<td>$\Delta m_{21}^2 [10^{-5} eV^2]$</td>
<td>7.54$^{+0.26}_{-0.22}$</td>
<td>6.99 - 8.18</td>
</tr>
<tr>
<td>$</td>
<td>\Delta m^2</td>
<td>[10^{-3} eV^2]$</td>
</tr>
<tr>
<td>$</td>
<td>\Delta m^2</td>
<td>[10^{-3} eV^2]$</td>
</tr>
<tr>
<td>$\sin^2 \theta_{12}$</td>
<td>0.308 ± 0.017</td>
<td>0.308 ± 0.017</td>
</tr>
<tr>
<td>$\sin^2 \theta_{23}$</td>
<td>0.437$^{+0.033}_{-0.023}$</td>
<td>0.374 - 0.628</td>
</tr>
<tr>
<td>$\sin^2 \theta_{13}$</td>
<td>0.0234$^{+0.0020}_{-0.0019}$</td>
<td>0.0176 - 0.0295</td>
</tr>
<tr>
<td>$\delta/\pi$</td>
<td>1.39$^{+0.38}_{-0.27}$</td>
<td>...</td>
</tr>
</tbody>
</table>

However, to determine the absolute neutrino masses, even though the oscillation parameters will plays an important part, other experiments are needed. For example, cosmological studies and beta decay experiments are setting limits on absolute neutrino masses as well as the sum of the masses, and are expected to improve these limits with future results [37].

Understanding how neutrino masses are generated plays an important part in the search for determining the masses. The masses of the other fermions in the Standard Model are generated by interactions with the Higgs field as Dirac fermions. By assuming the neutrino to also be a Dirac fermion, the masses can be generated using the Higgs mechanism via the Yukawa interaction. This results in an extremely small value of the neutrino Yukawa coupling, leading to the believe that there are more sources for neutrino mass generation [38]. A popular suggested solution to this is the seesaw mechanism, where we include a Majorana mass term in our Langrangian [39 40 38], based on the suggested Majorana particle by Ettore Majorana in 1937 [41]. An important property of a Majorana particle is that it is identical to its own antiparticle, breaking lepton number conservation
and making the process of neutrinoless double beta-decay possible, which we will explain in the next section.

2.4 Neutrinoless double beta decay \((0\nu\beta\beta)\)

The process of regular single beta decay in (2.2) can also be represented by the Feynman diagram in Figure 2.2. At the elementary level, this is an interaction where a down quark is converted into an up quark while emitting a \(W^-\) boson that subsequently decays into an electron and an antielectron neutrino. When this decay happens to a neutron within a nucleus \(\frac{A}{2}X\), it will change the nucleus by increasing its atomic number \(Z\) (number of protons) by one. The decay is allowed if the mass energy of the new nucleus \(\frac{A}{2}+1X'\) is lower than the mass energy of \(\frac{A}{2}X\), so that the difference

\[
Q = m(\frac{A}{2}X) - m(\frac{A}{2}+1X') - m(e^+) - m(\bar{\nu}_e)
\]

(2.6)

is positive. The energy given by the \(Q\)-value (2.6) is the combined kinetic energy of the decay products.

According to the semi-empirical mass formula (SEMF) of nuclear physics [42], the mass energy of a nuclei with odd mass number \(A\) (number of nucleons) will, as a function of the atomic number \(Z\), follow the shape of a parabola. An example of the left half of this parabola is shown in Figure 2.3a. Nuclei that are higher up on the parabola, i.e. with lower \(Z\) values, can transit to a lower energy level by the single beta decay process.

It is important to mention here that what we have been talking about until now is called the \(\beta^-\) decay process. There also exists a \(\beta^+\) decay process, which is analogous to \(\beta^-\) decay, where a proton decays into a neutron (down quark to up quark) emitting a positron \((e^+)\) and an electron neutrino \((\nu_e)\). This process reduces the atomic number \(Z\) and is allowed for nuclei in the right half of the SEMF parabola, i.e. higher \(Z\) values. For the same nuclei that allow \(\beta^+\) decay there is also a possibility for electron capture.
(K-capture) to occur. In the case of electron capture, the nucleus captures an electron and emits an electron neutrino, resulting with the atomic number of the nucleus reducing by one. The focus of the rest of this chapter will be on the $\beta^-$ decay processes.

In the case of a nuclei with an even mass number $A$ the situation is slightly different. For a nuclei with even mass number $A$ the mass energy levels, as a function of the atomic number $Z$, will follow two different parabolas. Nuclei with even mass number $A$ and even atomic numbers $Z$ are on a lower parabola then the parabola that the nuclei with even mass number $A$ and odd atomic number $Z$ will follow. In this case it is possible to get a situation like in Figure 2.3, where we have a nucleus $^{A-2}ZX$, with even mass number $A$ and even atomic number $Z$, having less mass energy than $^{A-1}ZX'$ but more mass energy then $^{2}X''$. For this nucleus, $^{A-2}ZX$, single beta decay is energetically forbidden.

On the other hand, the nucleus $^{A-2}ZX$ could decay to the lower mass energy level $^{A}X''$ by the double beta decay process, first proposed by Maria Goeppert-Mayer in 1935 [43]. Double beta decay ($2\nu\beta\beta$) is a nuclear process in which two neutrons decay into two protons at the same time and in the same manner as for single beta decay

$$^{A-2}ZX \rightarrow ^{A}ZX'' + 2e^- + 2\bar{\nu}_e,$$

(2.7)

represented by the Feynman diagram in Figure 2.4.

The first experimental observation of a $2\nu\beta\beta$ decay process, from the $^{130}_{52}$Te nucleus, was done in 1950 by Mark Inghram and John Reynolds [44]. The first direct observation of $2\nu\beta\beta$ decay, from the $^{82}_{43}$Se nucleus, was done by Elliott, Hahn and Moe in 1987 [45]. Currently, double beta decay has been observed in eleven isotopes, the measured half-lives of which are included in Table 2.2.

As stated earlier, a popular solution to understand the mass generation for neutrinos come from proposing that the neutrino is a Majorana particle, a particle that is identical to its antiparticle. As early as 1939 Wendell H. Furry applied the Majorana particle theory [23] to Goeppert-Mayer’s theory of double beta decay [43] and proposed that if the
Figure 2.4: Feynman diagram representing the double beta decay process.

Table 2.2: Compilation of recent reported measurements of double beta decay half-lives of known isotopes to undergo double beta decay. Most numbers are taken from [46].

| Isotope             | $T_{1/2}^{2
u\beta\beta}$ ($10^{19}$ yr) | Sources |
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Calcium-48</td>
<td>$4.4^{+0.6}_{-0.5}$</td>
<td>[47, 48, 49]</td>
</tr>
<tr>
<td>Germanium-76</td>
<td>$150 \pm 10$</td>
<td>[50, 51, 52, 53]</td>
</tr>
<tr>
<td>Selenium-82</td>
<td>$9.2 \pm 0.7$</td>
<td>[54, 55]</td>
</tr>
<tr>
<td>Zirconium-96</td>
<td>$2.3 \pm 0.2$</td>
<td>[56]</td>
</tr>
<tr>
<td>Molybdenum-100</td>
<td>$0.71 \pm 0.04$</td>
<td>[57, 58]</td>
</tr>
<tr>
<td>Cadmium-116</td>
<td>$2.8 \pm 0.2$</td>
<td>[49, 59, 60, 61]</td>
</tr>
<tr>
<td>Tellurium-128</td>
<td>$(2.41 \pm 0.39) \times 10^5$</td>
<td>[62]</td>
</tr>
<tr>
<td>Tellurium-130</td>
<td>$70^{+9}_{-11}$</td>
<td>[63, 64]</td>
</tr>
<tr>
<td>Xenon-136</td>
<td>$217 \pm 6$</td>
<td>[65]</td>
</tr>
<tr>
<td>Neodymium-150</td>
<td>$0.82 \pm 0.09$</td>
<td>[58, 56]</td>
</tr>
<tr>
<td>Uranium-238</td>
<td>$200 \pm 60$</td>
<td>[67]</td>
</tr>
</tbody>
</table>
neutrino is a Majorana particle then a double beta decay process, without the emission of neutrinos, could be possible [68]. In 1982 Schechter and Valle showed that the existence of this decay would imply that the neutrino has a Majorana nature [69].

This decay process is called neutrinoless double beta decay ($0\nu\beta\beta$) and it is described by the Feynman diagram in Figure 2.5. The process is similar to that of double beta decay, represented in Figure 2.4 except that the two emitted antielectron neutrinos have been replaced by an internal Majorana neutrino that is exchanged between the two $W^-$ bosons. This process is allowed, according to the Majorana fermion theory, despite the fact that we have an internal line, with arrows pointing in both directions, in Feynman diagram, because as Majorana particles the neutrino and the antineutrino are identical. Also, we see that this process breaks the conservation of lepton number because there are no antielectron neutrinos in the decay product, resulting in $\Delta L_e = 2$ after the process.

```
\[
\begin{array}{ccc}
  n & u & u \\
  d & d \\
  d & u \\
\end{array} \\
\begin{array}{c}
  p \\
  W^- \\
  W^- \\
  e^- \\
  e^- \\
  \nu_M \\
\end{array}
\]
```

**Figure 2.5:** Feynman diagram representing the neutrinoless double beta decay process.

As mentioned earlier, the decay products of single and double beta decay will have a combined kinetic energy equal to the $Q$-value of the decay, (2.6) on page 11. When measuring the combined kinetic energy of the emitted electrons from single and double beta decay, a continuous distribution of energies below the $Q$-value is expected, as in Figure 2.1 (page 7). This is because the antielectron neutrinos leave undetected with some of the kinetic energy. In the case of neutrinoless double beta decay, there are no antielectron neutrinos in the decay product, resulting in the two electron getting all the $Q$-value energy as kinetic energy. Measurements of the kinetic energy of the emitted electrons thus results in a peak at the $Q$-value of the decay, as shown in Figure 2.6.

Currently, no credible experimental evidence for neutrinoless double beta decay has been produced. However, a lot of experiments have set lower limits on the half-life of neutrinoless beta decay for different isotopes, presented in Table 2.3. Current and future
experiments are still searching for neutrinoless double beta decay. Among them is the SNO+ experiment, where the main goal is to detect neutrinoless double beta decay from Tellurium-130, which is the topic for the next chapter.

### 2.5 Neutrinoless double beta decay detection

There exist two general approaches for experimental investigations of double beta decay: indirect, or inclusive, methods and direct, or counter, methods. The first approach looks at anomalous concentrations of daughter nuclei in properly selected samples, and includes geochemical and radiochemical methods. Using this method makes it difficult to separate between regular double beta decay and neutrinoless double beta decay events, but it has played an important part in measurements of regular double beta decay half-lives.

Experiments that employ the direct, or counting, methods are using detectors to count direct observations of the two electrons that are emitted from a double beta decay. They then uses information from the detected electrons (energies, momenta, topology, etc.) to determine whether a set of electrons are likely to have been created by a regular double beta decay or a neutrinoless double beta decay, considering the signature signals visualised in Figure 2.6. The direct counting methods can further be subdivided into two groups: homogeneous methods, where the source material for the double beta decay is a part of the detector, and inhomogeneous methods, where the electrons originate from an external double beta decay source.

In the experimental search for neutrinoless double beta decay there are three important concerns that need to be addressed. Firstly, a very good energy resolution is required in order to identify the sharp peak of the neutrinoless double beta decay signal over the flat background, also taking into account the tail of the regular beta decay signal. Secondly, because of the low event rate expected from neutrinoless double beta decay, minimising the background rate as much as possible is an important task, prompting excellent shielding and radio-pure materials. Thirdly, measured neutrinoless double beta decay rates will depend on the amount of isotopes that can undergo the decay, so maximising the mass of the selected isotope is beneficial.

The goal of neutrinoless double beta decay experiments is to either measure the half-life of the decay, or to put an improved lower limit on the half-life. Theoretically the half-life, or more precisely the decay rate, of neutrinoless double beta decay is given by

\[
\Gamma^{0\nu\beta\beta} = \left( T_{1/2}^{0\nu\beta\beta} \right)^{-1} = G^{0\nu} \cdot |M^{0\nu}|^2 \cdot \frac{\langle m_{\beta\beta} \rangle^2}{m_e^2}.
\]
Figure 2.6: Spectrum of combined energy of electron pair for regular double beta decay (blue) and neutrinoless double beta decay (red). Plot taken from [70].

Table 2.3: Current experimental lower limits on neutrinoless double beta decay half-lives for isotopes that undergo double beta decay.

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$T^{0\nu\beta\beta}_{1/2}$ (10^{24} yr)</th>
<th>Sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>Calcium-48</td>
<td>&gt; 0.058</td>
<td>71</td>
</tr>
<tr>
<td>Germanium-76</td>
<td>&gt; 19</td>
<td>72</td>
</tr>
<tr>
<td></td>
<td>&gt; 15.7</td>
<td>73</td>
</tr>
<tr>
<td>Selenium-82</td>
<td>0.36</td>
<td>74</td>
</tr>
<tr>
<td>Zirconium-96</td>
<td>0.0092</td>
<td>56</td>
</tr>
<tr>
<td>Molybdenum-100</td>
<td>1.1</td>
<td>74</td>
</tr>
<tr>
<td>Cadmium-116</td>
<td>0.17</td>
<td>60</td>
</tr>
<tr>
<td>Tellurium-130</td>
<td>2.8</td>
<td>75</td>
</tr>
<tr>
<td>Xenon-136</td>
<td>1.6</td>
<td>76</td>
</tr>
<tr>
<td>Neodymium-150</td>
<td>0.018</td>
<td>66</td>
</tr>
</tbody>
</table>
$G^{\nu\nu}$ is the two-body phase-space factor, $M^{0\nu}$ is the nuclear matrix element of the $0\nu\beta\beta$ decay, and $m_{\beta\beta}$ is called the effective Majorana mass given as

$$\langle m_{\beta\beta} \rangle = \sum_k U_{ek}^2 m_k,$$

(2.9)

where $m_k$ is the neutrino masses and $U_{ek}$ is the neutrino mixing matrix. Theoretical calculations of the nuclear mixing element $M^{0\nu}$ are very difficult and, due to different calculation models giving different results, have large uncertainties [77]. Calculated phase-space factors for viable neutrinoless double beta decay isotopes are included in Table 2.4 along with $Q$-values, isotropic abundance and experiments using the isotopes.

Further information on neutrinoless double beta decay detection can be obtained from [46, 70].

Table 2.4: Phase-space factors, $Q$-values and isotropic/natural abundance for neutrinoless double beta decay candidate isotopes. Also lists past, present and future experiments using the different isotopes. Values reproduced from [78].

<table>
<thead>
<tr>
<th>Isotope</th>
<th>$G^{\nu\nu}$ [$10^{-15}$ yr$^{-1}$]</th>
<th>$Q_{\beta\beta}$ [keV]</th>
<th>I.A.[%]</th>
<th>Experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca-48</td>
<td>24.81</td>
<td>4272</td>
<td>0.187</td>
<td>CANDLES [79]</td>
</tr>
<tr>
<td>Ge-76</td>
<td>2.363</td>
<td>2039</td>
<td>7.8</td>
<td>GERDA [80], MAJORANA D. [81], MAJORANA D. [81], GEM [82], Heidelberg-Moscow [72], IGEX [73]</td>
</tr>
<tr>
<td>Se-82</td>
<td>10.16</td>
<td>2995</td>
<td>9.2</td>
<td>SuperNEMO [83], LUCIFER [84]</td>
</tr>
<tr>
<td>Zr-96</td>
<td>20.58</td>
<td>3504</td>
<td>2.8</td>
<td>-</td>
</tr>
<tr>
<td>Mo-100</td>
<td>15.92</td>
<td>3034</td>
<td>9.6</td>
<td>MOON [85], AMoRE [86], NEMO 3 [87]</td>
</tr>
<tr>
<td>Cd-116</td>
<td>16.70</td>
<td>2816</td>
<td>7.5</td>
<td>COBRA [88]</td>
</tr>
<tr>
<td>Te-130</td>
<td>14.22</td>
<td>2527</td>
<td>34.5</td>
<td>CUORE [89], CUORICINO [75], SNO+ [90]</td>
</tr>
<tr>
<td>Xe-136</td>
<td>14.58</td>
<td>2458</td>
<td>8.9</td>
<td>EXO [91], NEXT [92], KamLAND-Zen [93]</td>
</tr>
<tr>
<td>Nd-150</td>
<td>63.03</td>
<td>3371</td>
<td>5.6</td>
<td>DCBA [94]</td>
</tr>
</tbody>
</table>
Chapter 3

The SNO+ Experiment

3.1 General information on the SNO+ experiment

The SNO+ experiment is a multi-purpose neutrino experiment located at SNOLAB in Sudbury, Ontario in Canada. SNOLAB is a science facility located about 2 070 meters underground in the Vale’s Creighton nickel mine \[^{95,96}\]. It is an expansion of the Sudbury Neutrino Observatory (SNO), which is a solar neutrino experiment facility that contributed to the discovery of neutrino oscillations, as mentioned earlier \[^{34,35}\]. The facility provides shielding from cosmic rays, due to the about 6010 m.w.e \[^{1}\] shielding of the overburden rock. It is also an ultra-clean facility, which combined with the cosmic ray shielding, makes it ideal for experiments requiring high sensitivities and studies of rare interactions and decays.

The scientific work at SNOLAB is mainly focused on studies and detection of neutrino particles and dark matter detection experiments. Experiments that are currently running or under construction at SNOLAB are the HALO and the SNO+ neutrino experiments, as well as the dark matter detection experiments: DAMIC, PICO, DEAP, MiniCLEAN and SuperCDMS. Planned future experiments at SNOLAB are the next generation neutrino experiments nEXO and COBRA, and the dark matter detection experiment NEWS.

The SNO+ collaboration consists of about 140 scientists from 25 institutes, from Canada, USA, UK, Mexico, Portugal and Germany\[^{2}\]. The SNO+ project started in the middle of the last decade, as an idea of re-using the SNO experiment facility, replacing the heavy water with a liquid scintillator \[^{97}\].

The primary goal of the SNO+ experiment is the detection of neutrinoless double

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\[^{1}\] Meter water equivalent: shielding against cosmic rays equivalent to the shielding obtained at the given meters under the surface of water.

\[^{2}\] http://snoplus.phy.queensu.ca/People.html (Accessed: 05.05.16)
beta decay, specifically from the isotope tellurium-130 that is to be dissolved into the liquid scintillator. Tellurium-130 is the neutrinoless double beta decay isotope of choice because of its high natural abundance (see Table 2.4 on page 17), the possibility to suppress uranium and thorium backgrounds, the low background rates, no inherent atomic absorption for tellurium in the optical range, and the relatively low costs [98].

The SNO+ experiment also has a range of other scientific goals [90]. The experiment will attempt to detect low energy pep and CNO solar neutrinos. Neutrinos from the uranium and thorium decay chains in the Earth, called geoneutrinos, will be studied. Antineutrinos from nuclear reactors will be detected to study neutrino oscillations. SNO+ will be able to detect neutrinos and antineutrinos from galactic supernovae, and will be expected to participate in the Supernova Early Warning System (SNEWS) [99]. In addition, the SNO+ experiment will be able to study some other aspects of beyond the Standard Model physics, such as invisible nucleon decay and axion searches.

3.2 Technical specifications of the SNO+ experiment

The SNO+ neutrino experiment is the successor experiment to the SNO experiment, and will be re-using the experiment infrastructure and facilities used by the SNO experiment. The SNO+ experiment consists of a spherical 12 meter diameter acrylic vessel (AV) at the centre, which will be filled with 780 tonnes of liquid scintillator. Around the AV there is a 18 meter diameter geodesic sphere, called the PMT support structure (PSUP), that is made of stainless steel and contains about 9500 PMTs pointing inwards towards the AV.

The area between the AV and the PSUP will be filled with ultra-pure water acting as a shield against radiation from the PSUP and the surrounding rock. In addition, there is a system of ropes to keep the detector in place. The rope system consists of hold-up ropes, as used by the SNO experiment, and some new hold-down ropes, because the density of the liquid scintillator is lower than the density of water. A sketch of the SNO+ detector is given in Figure 3.1a along with an artistic view of the detector in Figure 3.1b.

The SNO+ experiment will consist of three main data taking phases. The first phase, the water-filled phase, is supposed to start during 2016 and will last for a few months. The acrylic vessel will be filled with 905 tonnes of ultra-pure water during this phase, which will focus on exotic physics and supernova neutrinos as well as testing of detector performance. According to a status report from early 2016 the experiment is now partially filled with ultra-pure water [90].

The second phase is the pure scintillator phase, where the AV will be filled with the
Figure 3.1: The SNO+ detector. The sketch (a), taken from [90], depicts the acrylic vessel (AV) in blue with the cylindrical neck extending up to the deck, the PMT support structure (PSUP) in green, the hold up ropes in purple and the hold down ropes in red. The same components can be seen in (b), except the hold down ropes since this is an artistic view of the old SNO detector.

scintillator liquid. The research focus for this phase will be on the measurements of solar, geo, reactor and supernova neutrinos, as well as studying and monitoring the detector performance. Thirdly, it is the Te-loading phase, where 2.3 tonnes of natural tellurium will be dissolved into the scintillator liquid (0.3% loading). This phase is called Phase I, and is the phase when the SNO+ experiment will focus on the detection of neutrinoless double beta decay. The Te-loading phase is projected to start in 2017 and will last for about 5 years.

The 780 tonnes of liquid scintillator chosen to be used for the SNO+ experiment will consist of linear alkylbenzene (LAB) with 2 grams per litres of 2,5-diphenyloxazole (PPO) [100]. Listed reasons for choosing LAB as the liquid scintillator are its long time stability, compatibility with the acrylic, high purity level, high light yield, linear response in energy and good particle identification capabilities [101]. The PPO will function as a wavelength shifter, in order for the emitted scintillator light to be in a wavelength region better suited for the PMTs. A processing plant for scintillator purification and liquid handling have
been designed and constructed for the experiment [102].

For the Te-loading phase the liquid scintillator will be loaded to 0.3% with tellurium, which will be dissolved into the scintillator, in the form of a purified telluric acid, by methods developed for this purpose [103, 104]. To further improve the detectors efficiency, a secondary wavelength shifter, not yet decided, will be added to better match the PMTs. Currently perylene and bis-MSB are investigated for this purpose, and will be selected on the basis of optical properties, light yield and scattering lengths for the full Te-loaded mixture.

The SNO+ detector uses the same original photomultiplier tubes (PMTs) used for the SNO detector, which are the 20.4 cm diameter Hamamatsu R1408 PMTs. These are equipped with a 27 cm diameter concentrator that increase the effective photocathode coverage of the experiment to about 54% [105]. A picture of a similar PMT from Hamamatsu is included in Figure 3.2.

![Figure 3.2: Picture of the photomultiplier tube Hamamatsu R5912.](http://lampes-et-tubes.info/pm/pm045.php?l=e (Accessed: 05.05.16)

Figure 3.2: Picture of the photomultiplier tube Hamamatsu R5912, taken from [3]. Looks similar to the Hamamatsu R1408 photomultiplier tubes used for the SNO+ experiment and the SNO experiment before.

The calibration system for the SNO+ experiment is based on optical sources, radioactive sources and cameras. The camera system will be used to monitor the position of the detector components, such as the acrylic vessel and the rope systems, as well as for position triangulation of calibration sources that are inserted into the detector. Different
radioactive materials will be inserted into the detector in order to check the energy scale, the energy resolution, the linearity of the response and the detector asymmetries. A range of material with radiation covering the range between 0.1 MeV and 6 MeV have been suggested for this purpose.

The optical calibration system consist of internally deployable sources, such as a laser ball (light diffusing sphere) and a Cherenkov source. Additionally, an external optical calibration system will be used. This will consist of light-emitting diodes (LEDs) or lasers that produce light that will be injected into the detector via fibres that are attached to the PMT support structure. The purpose of the optical sources will be used to check the PMT response, time and gain, and measure in situ the optical properties. Using the external optical calibration system the optical properties of the detector can be monitored frequently and without the need to insert external sources into the detector, minimising the risk of radioactive contamination of the detector.

Further information on the SNO+ experiment, its current status and future prospects, can be obtained from [90].

3.3 Embedded LED Light Injection Entity (ELLIE)

The external light injection system that will be used for the optical calibrations for the SNO+ experiment is called the Embedded LED Light Injection Entity (ELLIE) [106, 107]. ELLIE consists of a LED/laser based light generator located on the deck above the detector where it can be operated. The light then goes through a set of 47.75 metre fibres that runs from the light generator, down to the detector and into various injection points in the PMT support structure. A sketch of the ELLIE system is included in Figure 3.3.

ELLIE will consist of three subsystems based on the same principle but for different purposes. These are the Timing ELLIE (TELLIE) which will be used for timing calibrations and gain measurements of the PMTs. TELLIE will consist of 110 fibres that will enable all the PMTs in the PSUP structure to be illuminated. The LEDs that will be used for TELLIE have a mean peak wavelength at (505.6 ± 2.6) nm, and with a typical spread of 43% (RMS/mean). This is chosen to be within the range of the expected detectable light during the experiment, as well as to achieve low scattering probability in the liquid scintillator, while keeping the peak wavelength at a high quantum efficiency for the PMTs. The LEDs have a intensity range of $10^3$ to $10^5$ photons with a pulse width bellow 5 ns and a broad emission angle with 80° of light within a 14.5° cone from the centre of the beam.

The Scattering Module of the ELLIE (SMELLIE) is designed to monitor the optical
scattering properties of the liquid scintillator mix, and will be using the laser heads as light sources. SMELLIE will consist of 12 fibres connected at four different nodes (07, 25, 37, 55) and with an emission direction of either 0°, 10° or 20° with respect to the detector centre. Four pulsed-diode PicoQuant LDH Series laser heads will also be used for SMELLIE, with the wavelengths 375nm, 405nm, 440nm and 500nm. These laser heads have a 10kHz repetition rate and with very short pulses (<100ps).

The Attenuation Monitoring ELLIE (AMELLIE) is designed to monitor and measure attenuation lengths in the liquid scintillator mix. AMELLIE will consist of 8 fibres connected at four different nodes (89, 73, 50, 08), with two different available emission angles, 0° and 20° with respect to the detector centre. The LED light that will be used for AMELLIE is similar to the LED light used for TELLIE, except that it will have a gaussian angular distribution with $\sigma = 3.5^\circ$. Two different wavelengths are to be determined for the AMELLIE LED light. Locations of the AMELLIE fibre mount points are specified in Figure 3.5.
The optical fibres that will be used for ELLIE are connected to the LED/laser sources at the deck above the detector, inserted into the detector area by a feed-through box and then connected to mount points on the detector. These mount points are located at the nodes of the geodesic PSUP structure so as to give uniform coverage of all the PMTs and no shadowing on or from the PMTs. In Figure 3.4 the positions of the nodes are shown as designated numbers.

Figure 3.4: Position map of the geodesic nodes on the PSUP structure used for ELLIE fibre mounting points. This map is a 2D representation (folded out) of the spherical PSUP structure.

Figure 3.5: Positions (red circles) of the four fibre mount points used for the AMELLIE fibres on the PSUP structure. The node IDs are from left to right 89, 73, 08 and 50.
Chapter 4

Simulations with RAT

As mentioned earlier, this project is a study of how optical degradations on the liquid scintillator affects the SNO+ experiment by simulating the AMELLIE subsystem of the ELLIE calibration system. Simulations of different experimental conditions as well as different degrees of optical degradations on the scintillator materials have been preformed. Simulations of the AMELLIE system have been used for the study, because of the fact that AMELLIE will be used for the actual monitoring of the optical degradation during data taking. The purpose is then to make some benchmarks that can indicate possible optical degradations if certain deviations of intensities are measured by the AMELLIE calibration system. Additionally, the goal of the simulations is to obtaining an in depth understanding of the information from the AMELLIE measurement output.

4.1 Reactor Analysis Tool (RAT)

The simulations and analysis are performed by the use of the Reactor Analysis Tool (RAT) framework\textsuperscript{1}. RAT was originally developed by Stan Seibert for the Braidwood Collaboration\textsuperscript{2} to be a flexible, extensible and general-purpose simulation and analysis package for optical detectors. It is built with GEANT\textsuperscript{3}, for the command interpretations, ROOT\textsuperscript{4}, for the input/output features, CLHEP\textsuperscript{5}, for the physics software classes, and GLG4sim\textsuperscript{6} for Monte Carlo event production. The design of RAT is inspired by SNOMAN, the Monte Carlo simulation and analysis software developed for the SNO experiment. Currently, the RAT package is jointly developed by the SNO+,

\textsuperscript{1}http://rat.readthedocs.org/en/latest/ (Accessed: 06.05.16)
\textsuperscript{2}http://www.geant4.org/geant4/ (Accessed: 06.05.16)
\textsuperscript{3}https://root.cern.ch/ (Accessed: 06.05.16)
\textsuperscript{4}http://proj-clhep.web.cern.ch/proj-clhep/ (Accessed: 06.05.16)
\textsuperscript{5}http://neutrino.phys.ksu.edu/ GLG4sim/ (Accessed: 06.05.16)
MiniCLEAN and DEAP collaborations for the use in these specific experiments. Rat is also used by other experiments or collaborations, because of its flexibility and extensibility.

The purpose of the RAT framework is to enable simulations of a given experiment by defining the geometry of the experiment and detector in detail. RAT offers the option to modify the geometrical or optical properties of the defined detector, in order to study how various parameters or designs affect the experiment. With a given detector/experiment definition, RAT can be used to simulate realistic Monte Carlo-generated events corresponding to signals, backgrounds or calibration sources.

For the Monte Carlo events RAT offers the option to track event particles through a detailed detector environment, attempting to give as detailed information about the physics as reasonably achievable. RAT also offers a detailed modelling of the detector hardware, such as a internal PMT model, as well as simulating the digitisation, triggering and readout of simulated signals. Finally, RAT provides an analysis framework capable of analysing the Monte Carlo simulated events, as well as actual detector data, with only a few command changes. This enables both simulated and real data to be compared by RAT, using the same code and software.

A public edition of RAT is available on [GitHub](https://github.com/rat-pac/rat-pac) (Accessed: 06.05.16).

### 4.1.1 RAT simulation settings

RAT offers a range of settings for the simulations, that can be set and modified by a macro file or directly in RAT before initialising the simulations. Some of these settings are connected to a set of database files describing detector environments and their physical properties. The standard RAT distribution for the SNO+ experiment includes database files for various phases of both the SNO experiment and the SNO+ experiment. In the case of SNO+, the RAT distribution includes definitions of the SNO+ detector where the acrylic vessel is filled with air, water, scintillator or Te-loaded scintillator. Further, it is possible to change certain properties of these experiment definitions, such as the positioning of the different components, the materials of the components and the physical properties of the materials in use. Some of the defined RAT geometry for the SNO+ experiment is shown in Figure 4.1.

Important settings for ELLIE simulations in RAT relate to the position and emission direction of the fibre injection point, as well as the features of the light pulses emitted from the fibre. For simulations of ELLIE with RAT one must first specify which fibre

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6https://github.com/rat-pac/rat-pac (Accessed: 06.05.16)
Figure 4.1: Visualisation of PSUP structure in green (a) and the AV in blue (b), based on the SNO+ geometry definitions in RAT. Both figures show the hold-up and hold-down ropes, blue lines in (a) and red in (b). The grey tube at the top of both images is called the neck. Images taken from an internal SNO+ document.

injection point to use. The light pulse features include the light intensity, the wavelength distribution, the time distribution and the angular distribution of the pulse. Additionally, the number of events, which corresponds the number of pulses, in the ELLIE simulations are given before initialisation. The number of events ultimately determines the statistics of the simulations.

4.1.2 RAT simulation output

The input and output handling in RAT is done using the ROOT formalism. As a consequence of this, the output of the simulated data is structured in the form of a TTree object in a ROOT data file. Along with this, one also obtains a log file from the simulations, which contains important information about the simulation and how it progressed. The way the simulation data is stored in the ROOT file structure is in the form of different branches in the TTree structure, each containing information on different aspects of the simulation. These are the \texttt{mc} branch, containing information on the Monte Carlo simulated particles, the \texttt{mcevs} branch, containing the detected events as defined by the trigger simulations, the \texttt{evs} branch, containing the detected information of events that mimics how “real life” data would look like, and the \texttt{headerInfo} and \texttt{calib} branches, containing
additional information on the events and information about the potential active calibration sources.

4.1.3 RAT simulation tracking

If particle tracking has been enabled for the simulations, the mc branch in the ROOT output file also includes tracking information about the event particles in the simulations. The contents of the tracking information gives a detailed description of what happens to particles or light that are going through the detector before eventually being detected. Specifically, in the case of photon tracking, the tracking information describes how the light passes through different materials, indicating whether the light is reflected or transmitted, and whether the light is scattered, absorbed or re-emitted in the detector material. In addition, information on position, time, momentum, polarisation and kinetic energy along the path can be inferred from the tracking information. In the case of simulations of the ELLIE calibration system, the tracking information describes the path of the fibre injected light.

RAT provides some tools and utilities which can be used to extract specific information about particles, events, geometry or detector components, that can be used for further analysis of the simulated data. For the project described in this report two specific utilities are used: the RAT::DU::PMTInfo, which is used to extract information about a specific PMT, such as its position information, and the RAT::DU::LightPathCalculator, which is useful when studying the light path through the detector.

Two examples of the details that can be extracted from tracks describing photons in an AMELLIE simulation are included in Figure 4.2 and Figure 4.3. The first example, Track nr 241, in Figure 4.2 describes an optical photon that has been emitted from the LED injection point. This can be seen from the fact that the Parent ID of the track is 0. Also, the track starts in the cavity with an unknown status and by an unknown process, which is characteristic for an injected photon. The track is 11.54 meters long, and consists of 5 track steps, that represent different stages of the track.

Typically, a new track step is generated when something “happens” to the photon, most often this is the case when the light is reflected or transmitted through a geometrical boundary between two components or materials in the detector. Physical processes such as absorption, scattering or interactions with the PMTs also results in new track steps. Each track step contains information such as position, track step length, the status of the track and the process that the track step is describing. The Track Summary of the tracks
states the physical processes that the track has been through. For the Track nr 241, the Track Summary specifies that the track has undergone Rayleigh scattering in the liquid scintillator in the AV, and that the photon undergoes optical absorption inside the liquid scintillator at the end of the track.

The second example, Track nr 242, in Figure 4.3 describes an optical photon that is re-emitted from inside the liquid scintillator in the AV. This is affirmed from the fact that the track starts in the inner AV volume, and because the Summary Track states that the track has been through optical re-emission. Additionally, it can be concluded that the track describes a secondary photon, because of the fact that the Parent ID is non-zero. It turns out that the parent track of Track nr 242 is the first track example, Track nr 241, making it the initial photon. Track nr 242 has a length of 7.21 meters, and consists of 8 track steps. The track undergo Rayleigh scattering in the liquid scintillator in the AV before it ends by hitting a PMT.

The analysis of the two examples in Figure 4.2 and Figure 4.3 show how detailed tracking information can be used to follow and understand the path of an optical photon that is emitted from a fibre, absorbed in the AV, re-emitted, Rayleigh scattered and then ends by hitting a PMT.

4.2 Understanding simulations and simulation output

Since the focus of this project is to simulate AMELLIE events, this section will present some basic simulation results of the AMELLIE calibration system. The simulation used in this section is of 10 000 light beams (events) that are injected into the SNO+ detector from a AMELLIE fibre at the fibre node with ID number 73 (see Figure 3.5 on page 24). For this simulation, the experiment is in the liquid scintillator phase. The LED light used for the simulation has a wavelength distribution with a mean of 434 nm. The RAT macro used to initiate this simulation is given in Code A.1. It is important to note that the fibre ID set by the code is FA092, and not FA073. This is because the FA092 fibre had to replace the FA073 fibre in the node 73 fibre injection point.

The first aspect that will be studied is the intensity distribution of the photon beam, which in the simulation was set to 3000 with a Poisson pulse mode. Number of generated photons per pulse for the 10 000 pulses can be collected from the ROOT output file. The results for this data is presented by the histogram in Figure 4.4. The histogram shows how the intensity data fits with a Poisson distribution.

Next, in Figure 4.5 a histogram presenting the number of hit PMTs per photon pulses
Figure 4.2: Example of detailed tracking output from an AMELLIE simulation, describing light emitted from fibre.

Figure 4.3: Example of detailed tracking output from an AMELLIE simulation, describing re-emitted light.
in the simulation. The purpose of showing these two histograms together is to give an example of some easy accessible data from the simulation, which demonstrates what goes into the detector and what is actually measured in an AMELLIE scenario during the liquid scintillator phase. Allowing for multiple photon hits on a hit PMT, at least 4.4\% of the injected photons was detected by the PMTs.

Another way of studying the emitted photons and the PMT hits is by looking at their respective time distributions. A histogram of the simulated time distribution of the emitted photons is included in Figure 4.6 which in the simulation macro was set as a Gaussian distribution around $t = 0$ ns and with a standard deviation of $\sigma = 3$ ns.

On the other hand, collecting the PMT hit times in the simulation, results in the histogram presented in Figure 4.7. This histogram has an interesting shape, with a clear peak at around $t = 335$ ns but a weak, but somewhat evenly distributed, intensity in the time range 270-420 ns, and with a clear edge at $t = 420$ ns. From a quick analysis based on a general understanding of the detector, the clear peak at $t = 335$ ns represents the beamspot, which is light that goes straight through the detector and hits the PMTs on the opposite side of the fibre injection point. The signals that are somewhat evenly distributed in time represents light that is reflected against various surfaces through the detector, as well as from Rayleigh scattering and re-emission inside the liquid scintillator in the acrylic vessel.

In Figure 4.7, the time values on the x-axis do not represent the times between the emission of the photons and the time it hit the PMTs. Since RAT simulations also simulate the detector in detail, the time values also includes various processes in different detector components as well as the time of flight. Taking this into account, the time values of the time stamps for PMT hits should be viewed as relative times in the scope of this report.

The four histograms discussed above are a good way to start off our degradation study, because the goal of this project is to be able to understand what is happening to the injected photons inside the detector that causes the effects of the PMT readouts presented by the histograms. While the histograms on page 32 and 33 only contains information about the simulated light injection and detector output, in order to understand what is happening with the photons inside the detector it is helpful to look at the tracking information.

Considering what kind of information that can be extract from the tracking information of the simulations, it can be useful to look back at the tracking information examples in Figure 4.2 and Figure 4.3. An important aspect of our discussion of these examples was
Figure 4.4: Histogram of the simulated beam intensity from an AMELLIE fibre during the pure liquid scintillator phase. The black curve is a Poisson fit of the histogram.

Figure 4.5: Histogram of number of PMT hits in a pure liquid scintillator phase simulation with AMELLIE light injection.
Figure 4.6: Histogram of the simulated injection times of the photons emitted from a AMELLIE fibre in a simulation of the pure liquid scintillator phase. The line is a Gaussian fit of the data.

Figure 4.7: Histogram of the time stamps of the PMT hits in a pure liquid scintillator phase simulation of AMELLIE light injection.
how the tracks could be distinguished as light emitted from the fibre, or as re-emitted light from within the detector. Figure [4.8] presents a histogram of the different processes at the start of each track in the simulation. The track process “unknown” is characteristic for tracks starting at the fibre end. For this simulation, with 10 000 beams with a beam intensity averaging 3 000, there are about 30 million emitted photon and about 2.6 million re-emitted photons. This gives us some bearing on how many of the simulated photons are primary and secondary photons in this specific simulation.

The next interesting aspect of the tracking information is how the tracks end. This can be inferred from looking at the process at the end of the tracks, which is presented in the histogram in Figure [4.9]. First, the histogram shows that about 10.5 million of the photons are optically absorbed, of which only 2.6 million gets re-emitted, see Figure [4.8]. From this it can be concluded that from optical absorption about 7.9 million of the photons are “lost”, which amounts to about 24% of the initial and re-emitted photons in the simulation.

Further, about 11.7 million of the photons hit the PMTs, but not necessarily causing a hit, while the remaining 10.3 million photons end by the “Transportation” process. The “Transportation” process indicates that the photon passes through a geometrical boundary. When this causes the track to end it means that the track has left the detector. This makes sense because, as stated in Chapter [3], the SNO+ experiment has an effective photocathode coverage of about 54%. By considering only the tracks that hit a PMT and the tracks that leave the detector, the PMT hits make up about 53% of the tracks.

Finally, the histogram in Figure [4.10] presents the detector volume where the simulated tracks end. To understand this histogram the bin labels require an explanation. The bin label “av” indicates is the acrylic vessel itself, while the “inner_av” is the liquid scintillator contained by the AV. The “inner_PMT_pmt” and “innerPMT_concentrator” volumes are the end volumes that constitute a PMT hit. Next is the “world” and the “innerPMT_bucket” volumes, which is the area of the PMT environment that do not cause a photocathode hit. Tracks that end in both of these volumes corresponds to photons that are leaving the detector. Finally, there is the “cavity” volume, which is the area around the PSUP structure that is filled with water, the “hold_downropes” and the “hold_up_ropes”, and “Others”, which are various other detector volumes.
Figure 4.8: Histogram of the processes that causes new tracks in a pure liquid scintillator phase AMELLIE simulation. “Unknown” is the process that is characteristic for initially injected photons. The different types of “Reemission_from_comp” corresponds to primary and secondary reemission.

Figure 4.9: Histogram of processes that ends tracks in a pure liquid scintillator phase AMELLIE simulation. “OpAbsorption” means that the photon is optically absorbed. “G4FastSimulationManagerProcess” is the process that occurs when a photon hits a PMT. “Transportation” means that the photon passes through a geometrical boundary.
Figure 4.10: Histogram of the detector volumes where the photon tracks end in an AMEL-LIE simulation of the pure liquid scintillator phase.
Chapter 5

Visualisations and Classifications

In the previous chapter an example RAT simulation of AMELLIE was presented, and some basic information that can be extract from such simulations was shown. However, in order to properly study optical degradations of the scintillator material in the SNO+ experiment, a deeper understanding of the simulations and the tracking data is required. To achieve this, various ways of visualising the simulated data will be presented in this chapter. These visualisations will use both the time and the position information of the simulated signal detections to get a deeper understanding of the simulation output.

The two main ways of visualising the data, which will be presentation in detail in the following sections, are the PSUP hit map and the residual time vs. \( \cos(\theta_{\text{wrfp}}) \) hit map. Briefly explained, the PSUP hit map is a 2-dimensional map of the PMT support structure (PSUP), which indicates the number of PMT hits at various points around the PSUP structure. The residual hit time vs. \( \cos(\theta_{\text{wrfp}}) \) hit map is a 2-dimensional map, which indicates the number of PMT hits with respect to position and hit time of the PMT. The abbreviation “wrfp” in \( \theta_{\text{wrfp}} \) stands for with respect to the fibre position. The meaning of residual time and \( \theta_{\text{wrfp}} \) will be explained in Section 5.2.

5.1 PMT support structure (PSUP) hit map

In Chapter 4 when tracking information was discussed, it was also mentioned that RAT contained some useful utilities that could be used to analyse the simulation data. One that was mentioned, the `RAT::DU::PMTInfo` data utility, enables the extraction of the position of a specific PMT. When a hit PMTs is accessed from the evs branch, the `PMTInfo` utility returns a 3-dimensional vector of the position of the specific PMT in a Cartesian coordinate system. In the coordinate system the Z-axis points along the neck of the detector and in
the direction of the deck above the detector, see Figure 3.1 on page 20. The origin of the system is the centre of the detector and of the acrylic vessel.

Considering that all the PMTs are attached to the spherical PSUP structure it is convinient to view the hit PMT positions in a 2-dimensional hit map corresponding to how the fibre mount point positions are presented in Figure 3.4 (page 24) and in Figure 3.5 (page 24). To acheive this, a way to project the 3-dimensional Cartesian coordinates onto the 2-dimensional PSUP plane is needed. For this purpose, a C++ function called `psup_proj.cc` (Code A.2) is used, which is based on the position calculations of the vertices in a icosahedron\(^1\). This function takes a 3-dimensional Cartesian vector and projects it onto a 2-dimensional vector corresponding to the coordinates in the PSUP panel map.

Figure 5.1 contains a plot of the PSUP hit map of the same simulation data that was generated by the RAT macro in Code A.1 and that was studied in Chapter 4. The beamspot can be clearly seen as the high intensity region (red) at node ID 50, see Figure 3.4 (page 24), which is the diametrical opposite node to the fibre injection node that was used for the simulation.

At the fibre injection point at node ID 73 a concentration of hits (yellow) can be seen. This concentration is about two orders of magnitude lower than for the beamspot, but one order of magnitude larger than the elsewhere in the detector. Also, a larger area around the fibre injection point with a larger intensity than elsewhere. This larger concentration at and around the fibre injection point is due to reflections against the acrylic vessel and from the other side of the PSUP structure. The PMT hit intensity that is distributed across the detector (turquoise) is a combination of Rayleigh scattered and re-emitted light, as well as detector noise.

The benefits of using the PSUP hit map is that it shows how the PMT hits are distributed across the PMT support structure. It also clearly show the location of the beamspot, as well as indicating reflections back to the injection point. Still, the PSUP hit map lack some information from the simulation that could be useful in our further analysis. For example, the higher intensity around the injection point indicates reflected light, but it does not contain any information about when and where the light was reflected. These reflections could, as previously stated, be reflections against the acrylic vessel at the near side, before the light entered the liquid scintillator, the far side of the acrylic vessel, or against the PSUP structure on the opposite side of the detector. Also, in the discussion

\(^{1}\)http://www.rwgrayprojects.com/rbfnotes/polyhed/GeometricData/Icosahedron/Icosahedron.pdf
(Accessed: 08.05.16)
Figure 5.1: PSUP hit map for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.

On Figure 4.7 (page 33) in Chapter 4, it was stated that the edge at $t = 420$ ns could be due to reflections against the PSUP structure on the opposite side of the detector from the injection point.

5.2 Residual time vs. $\cos(\theta_{wrfp})$ hit map

As a complement to the PSUP hit map, and as a way of including the time information of the hit PMTs, this section will present another way of visualising the simulation data. From the simulation data of the hit PMTs in the evs branch the time stamp for the PMT hit can be extract, as was done in Chapter 4. As in the case of the PSUP hit map, it is beneficial to view the simulated data in a 2-dimensional intensity plot. With the timing information as a new parameter, in order to get a 2-dimensional intensity plot, a way of describing the position of hit PMTs by one parameter is needed.

Assuming that the light beam from the fibre is symmetric around the axis of its direction of emission, and that the detector itself is more or less spherically symmetric with respect to it centre. Also, considering that the AMELLIE fibres that inject light straight towards the detector centre are used, not the ones that inject light at a $20^\circ$ angle. Then,
it can be expected that the beam intensity detected at PMTs that have the same angle $\theta_{\text{wrfp}}$, with respect to the fibre position from the centre of the detector, will be the same or at least very similar.

Figure 5.2 gives a graphical definition of the angle $\theta_{\text{wrfp}}$. Continuing, the value $\cos(\theta_{\text{wrfp}})$ will be used as a parameter to describe the position of the hit PMTs from the simulation results. Not all of the assumptions stated above applies when using the fibres that emits the light at an $20^\circ$ angle, with respect to the centre of the detector. But, in this case, the angle $\theta_{\text{wrfp}}$ or the measure $\cos(\theta_{\text{wrfp}})$, can still be used, keeping in mind that the same assumptions does not apply.

Now that a parameter that describes the position of the hit PMT has been defined, it can be combined with the time stamp of the PMT hits in order to construct an intensity hit map for the position and time of PMT hits. This has been done for the AMELLIE simulation data created by the RAT macro in Code A.1 and is presented in Figure 5.3.

By looking at the time development along the $y$-axis, initially the near side AV reflections can be seen at $t \approx 280$ ns and located at around $\cos(\theta_{\text{wrfp}}) = 1$, which corresponds to the area close to the light injection point. Between $t \approx 280$ and when the beamspot appears, it looks like, as the beam moves through the detector, light of low intensity (turquoise) are scattered across the detector, gradually appearing for lower $\cos(\theta_{\text{wrfp}})$ values as time increases.

At the time $t = 335$ ns the beamspot appears (red) for $\cos(\theta_{\text{wrfp}}) \in [-1, -0.9]$, which is on the opposite side of the detector from the fibre injection point. Later, at $t \approx 370$, a weak intensity peak (yellow) appears at the beamspot location, which might be due to reflections of the initial beam against the PSUP structure and then again against the AV back to the PMTs. A back of the envelope calculation of the time of flight for light in vacuum back and forth between the PMTs and the AV (3m+3m) is about 20 ns, so this might be correct.

Finally, there are some weak intensity peaks between $t = 390$ ns and $t = 420$ for $\cos(\theta_{\text{wrfp}}) \in [0.4, 1]$, which likely is the reflections of the main beam that have travelled across the detector and has been reflected against either the far side of the AV or against the PSUP structure on the other side of the fibre injection point. With respect to time, these intensity peaks corresponds with the intensity edge discussed on the histogram in Figure 4.7 (page 33) in Chapter 4. The dark blue intensity region for times lower than $t = 300$ is from detector noise.

There is still some information that is missing in the Time vs. $\cos(\theta_{\text{wrfp}})$ hit map.
Figure 5.2: Graphical definition of the $\theta_{wrfp}$ angle. The outer circle represents the PSUP structure, the inner circle represents the acrylic vessel that contains the scintillator mix (blue). The black dot in the middle of the AV represent the centre of the detector.

Figure 5.3: Time vs. $\cos(\theta_{wrfp})$ hit map for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.
This comes from the fact that some photons might scatter multiple times in the liquid scintillator or is reflected multiple time inside the detector before being detected. As a consequence of this, two photons detected at the same time and at the same location might have taken different paths and been through different physical processes. This can be taken into account by introducing the new time parameter called \( t_{res} \). \textit{Residual time} is the difference between the time stamp \( t_{ts} \) of the event and the time of flight \( t_{sp} \) for a photon going in a straight path from the fibre to the hit PMT. The mathematical definition of \( t_{res} \) is given in \( (5.1) \).

\[
t_{res} = t_{ts} - t_{sp}
\]  

(5.1)

The straight path between the fibre and a PMT often consists of the different materials of the different detector components of the SNO+ detector. Most of the time this is the liquid scintillator material inside the AV, the acrylic of the AV and the ultra-pure water between the AV and the PSUP structure. These materials each have a refractive index \( n_{\text{material}} \), that can be extracted for a photon of a specific kinetic energy \( KE \) by using the \texttt{RAT::DU::LightPathCalculator} utility in RAT. The \texttt{LightPathCalculator} can also be used to extract the distance \( d_{\text{material}} \) that a photon, which is going in a straight path between a fibre and a PMT, passes through a specific material. With this information about the straight path between the fibre injection point and the PMT, the time of flight \( t_{sp} \) for a photon going in a straight path can be calculated using

\[
t_{sp}(\text{fibre, PMT, } KE) = \frac{1}{c} \left( \sum_{\text{material}} d_{\text{material}} \cdot n_{\text{material}} \right),
\]  

(5.2)

where \( c \) is the speed of light in vacuum. The code excerpt in Code \A.3\ contains how the calculation of the \textit{residual time} \( t_{res} \) is implemented in the ROOT/C++ scripts used for the analysis.

Replacing the time stamp with the residual time \( t_{res} \) results in the residual time vs. \( \cos(\theta_{\text{wrfp}}) \) hit map presented in Figure \ref{fig:residual_time_hit_map}. In this hit map the beamspot appears at \( t_{res} \approx 250 \), because most of the photons that cause the beamspot hits goes straight through the detector before hitting the PMTs at the other end. Compared to the beamspot, the near side reflections comes slightly later in the residual hit time. This is because the near side reflections against the AV are hitting PMTs that are located close to the fibre injection point.

On the other hand, the far side reflections appear differently in the residual hit time picture than they did in the time picture. This is indicating how the reflected photons that cause the different intensity peaks might have travelled through the detector differently.
Figure 5.4: Residual time vs. \( \cos(\theta_{\text{wrfp}}) \) hit map for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.

When looking at the residual time hit map, it is important to remember that for higher values of \( t_{\text{res}} \), the more photons that caused the hits have moved around in the detector before being detected.

By introducing time into our hit maps, similar events can to a larger degree be distinguished, like reflections against the near AV, the far side AV or the PSUP structure. It is also shown that by choosing a suitable set of parameters, more details can be inferred from the simulated detector output, which corresponds to the detector output that will be measured by the actual calibration system.

### 5.3 Classifications of simulated PMT hit data

In this section the different types of PMT hits studied in Section 5.2 will be distinguished based on the tracking information of the tracks that cause the PMT hits. All tracks that represents photons that does not cause detected PMT hits are not included in the following study, because the focus is on signals that can be measured by the calibration system. These specific tracks are identified by first selecting one of PMTs from the \texttt{evs} branch that registered a hit, then check in the \texttt{mc} branch for the number of simulated photoelectrons (PEs) simulated in the PMT. Then for each of PEs in the specific PMT it is checked in the \texttt{mc} branch whether it is noise or if it can be related to a photon...
track. In the case of zero photoelectrons the PMT signal is marked as noise. ROOT/C++
implementation of this procedure is given in Code A.3.

With a procedure to identify the photon tracks that cause signals in place, the tracking
information, containing detailed descriptions on the path of the photons, can be accessed.
In order to define a set of categories by which these photon tracks will be classified, an
defining aspect of the tracking information, that can be used to distinguish the different
types of tracks, is selected. This aspect is the Track Summary of the photon tracks, see the
end of the two examples in Figure 4.2 and Figure 4.3, which contains general information
on the nature of the tracks. For example, various “flags” in the Track Summary indicates
whether the track hit the PMT and how it hit the PMT, if it has been through Rayleigh
scattering and where in the detector the scattering happened, and if it is an absorbed or
re-emitted track. A track might contain one or more of these “flags”. In the next section,
Section 5.3.1 the meaning of the different “flags” that appear in the Track Summary is
explained.

5.3.1 Track Summary flags

The selected tracks that cause signal all contains either the HitPMT flag or the HitConc
flag in the Track Summary. Both flags indicates that the photon hits a PMT, but the
difference is in the way the photon hits the PMT. The difference originates from the way
the PMTs are defined geometrically in the RAT simulations, see Figure 5.5. The light
blue structure in the figure is the actual photomultiplier tube, which is what the photon
has hit if it carries a HitPMT summary flag. A HitConc summary flag indicates that
the particle has hit PMT via the PMT concentrator. In the geometrical definition, the
PMT concentrator is the grey circle around the PMT in the frontal view, and the black
structure at the front of the PMT in the side view.

Further, if a track contains the OpAbsorption flag, it indicates that the photon was
absorbed at the end of the track. Optical absorption causes the track to end somewhere in
the detector, such as the AV, the liquid scintillator mix or the ultra-pure water. Depending
on what material the track was absorbed within, there is a certain probability that a re-
emitted light appear. The re-emitted light is described by a new track that is labeled as
the child track of the absorbed track. This new track will contain the OpReemission
flag in its Track Summary.

Finally, if a tracks contains the OpRayleigh flag, it describes a photon that experi-
enced Rayleigh scattering somewhere along its path. The detector volume within which
Figure 5.5: How the geometry of the PMTs are defined in RAT for the Hamamatsu R1408 photomultiplier tubes used for the SNO+ experiment. The view on the left is from the side of the PMT while the view on the right is from the front of the PMT.

the Rayleigh scattering occurred is specified by an additional flag in the Track Summary. These are the \texttt{OpRayleighH20} flag, for scattering in the ultrapure water between the PSUP structure and the AV, the \texttt{OpRayleighAV} flag, for scattering in the acrylic material of the AV, and the \texttt{OpRayleighInnerAV} flag, for scattering in the liquid scintillator mix contained by the AV.

5.4 Classification categories for signal events

A set of classification categories for tracks that cause signal hits is defined based on the various Track Summary flag described in Section 5.3.1. The categories and their definitions are listed below. It is important to note that the \texttt{HitPMT} and \texttt{HitConc} categories uses the same name as the Track Summary flag of the tracks they contain. In order to avoid confusion later in the text, it will be specified whether it is the category or the Track Summary flags that is mentioned. How the category definitions is implemented in ROOT/C++ is included in Code A.3.

\textbf{HitOther} All the tracks in the \texttt{evs} branch that causes a detected signal. This is the tracks that contains either of the summary flags \texttt{HitPMT} or \texttt{HitConc} as well as any \texttt{Other} Track Summary flags.

\textbf{HitPMT} Only tracks that either goes straight through the detector or that are reflected inside the detector, before ending as a direct hit on a PMT. This is the tracks that only contains the \texttt{HitPMT} Track Summary flag, and no other flags.
**HitConc** Only tracks that either goes straight through the detector or that are reflected inside the detector, before ending by hitting the PMT via the PMT concentrator. This is tracks that only contains the **HitConc** Track Summary flag, and no other flags.

**Hit** Only tracks that either goes straight through the detector or that are reflected inside the detector, before ending as a detected PMT hit. Contains either only the **HitPMT** or only the **HitConc** Track Summary flags, and no other flags. This category is a combination of the categories **HitPMT** and **HitConc**.

**HitOpReemission** Tracks that are re-emitted from somewhere in the detector before causing a detected signal. This is tracks that contains the Track Summary flag **OpReemission** as well as any other flags.

**HitOpRayleigh** Tracks that have undergone optical Rayleigh scattering before causing a detected signals. This is tracks that contains the Track Summary flag **OpRayleigh** as well as any other flags.

**HitOpReemRay** Tracks are re-emitted and have undergone optical Rayleigh scattering before causing detected signals. This is tracks that contains both the **OpReemission** and the **OpRayleigh** Track Summary flags as well as any other flags.

**Noise** PMT signals that is not related to any photoelectrons or photon tracks.

It is important to notice that the categories mentioned above are not mutually exclusive. The relation between the categories is mathematically given as

\[
\text{SIGNALS} = \text{HitOther} + \text{Noise}
\]

\[
\text{HitOther} = \text{Hit} + (\text{HitOpReemission} \cup \text{HitOpRayleigh})
\]

\[
\text{Hit} = \text{HitPMT} + \text{HitConc}
\]

\[
\text{HitOpReemRay} = \text{HitOpReemission} \cap \text{HitOpRayleigh}
\]

Figure 5.6 contains an Euler diagram of the relations between the different categories.

The different classification categories can now be presented by the PSUP and the residual time vs. \( \cos(\theta_{wrfp}) \) hit maps. Figure 5.7 presents the PSUP hit map of **Hit** category events. The beamspot region appears unchanged compared to Figure 5.1 (page 39). On the other hand, the intensity is about two order of magnitudes lower for the PMT hits that are not located in the beamspot or in the area around the fibre injection...
Figure 5.6: An Euler diagram of the relations between the different classification categories for signal events. All the grey fields indicates signal events, with everything on the left side of the vertical line corresponding to signals caused by photons (HitOther).

point. The reduced intensity is due to the exclusion of signal events where the photons are scattered or re-emitted.

Focusing on the intensity area around the fibre injection point in Figure 5.7, it appears as the intensity falls off slowly going away from the fibre injection point until a certain radius, where a ring of higher intensity is located. The intensity peak located at ring appears only the HitConc category hits, while intensity region close to the fibre injection point appears only for the HitPMT category hits. The reason for the difference of the HitPMT and the HitConc categories is because of the geometry definition of the PMTs in RAT, see Figure 5.5 (page 45). After the light has been reflected and refracted at various surfaces inside the detector it approaches the PMTs at different angles, which results in more direct PMT hits or more PMT hits via the concentrator depending on the angle of approach.

Further, the PSUP hit maps for the classification categories HitOpReemission and HitOpRayleigh are presented in Figure 5.9 and Figure 5.10 respectively. For the PSUP hit map of the HitOpReemission category, Figure 5.9, the intensity of the re-emitted light is almost isotropically distributed across the detector, except for an area around the beamspot location and the fibre injection point where a slightly higher intensity is observed.

This is because of the fact that most of the photons in the pulse follow a path from the fibre injection point straight across the detector to the beamspot, and that photons are absorbed and re-emitted along this path, see Figure 5.8. Assuming that the photons are re-emitted isotropically, a higher intensity of re-emitted photons close to the fibre injection
Figure 5.7: PSUP hit map of Hit category events for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.

The same effect appears to be the case for the Rayleigh scattered hits in Figure 5.10. However, the full explanation for this also includes the fact that the intensity $I$ for Rayleigh scattering is depend on the scattering angle $\theta$. This results in a larger intensity of forward and backward scattering as opposed to perpendicular scattering.

$$I = I_0 \frac{8\pi^4 N\alpha^2}{\lambda^4 R^2}(1 + \cos^2 \theta), \quad (5.3)$$

where $\lambda$ is the wavelength, $\theta$ the scattering angle, $N$ the number of scatterings, $\alpha$ the polarisation and $R$ the distance from the scattering location.

Finally, the different classification categories are presented by the residual time vs. $\cos(\theta_{wrfp})$ hit map. Figure 5.11 and Figure 5.12 contains the residual time vs. $\cos(\theta_{wrfp})$ hit maps for the HitPMT and the HitConc categories respectively. The intensity in the beamspot area is similar for both figures. This is also the case for the reflections from
Figure 5.8: Sketch of re-emission along the straight path from the fibre injection point to the beamspot location in the SNO+ experiment

the AV reflections at the beamspot area, which happens about 30 ns after main beamspot, as well as the near side AV reflection at around light injection point.

On the other hand, difference between the two categories appear for the far side reflections that hit PMTs located in the area around the fibre injection point. This is related to the discussions on Figure 5.7 (page 48) about the intensity regions of the HitPMT and the HitConc category hits. The HitPMT category hits are located at about $t_{res} = 370$ ns and $\cos(\theta_{wrfp}) \in [0.4, 0.8]$, and consists of light that is reflected against the far side of the acryllic vessel. The HitConc category hits are located at about $t_{res} = 400$ ns and $\cos(\theta_{wrfp}) \in [0.7, 1.0]$, and consists of light that is reflected against the far side of the PSUP structure.

Figure 5.13 and Figure 5.14 presents the residual time vs. $\cos(\theta_{wrfp})$ hit maps for the HitOpReemission and the HitOpRayleigh categories respectively. These figures shows that the re-emitted and Rayleigh scattered PMT hits are spread out across the detector at all times. The intensity of these PMT hits are highest early on and falls of for higher residual time. This is because of the fact that the amount of photons in the light pulse decrease over time as photons hit the PMTs or are absorbed by the material in the detector. Also, the higher inensity at the beamspot area and around the fibre injection area that was discussed in Figure 5.9 and Figure 5.10 can be observed. Additionally, the residual time vs. $\cos(\theta_{wrfp})$ hit map for Rayleigh scattered PMT hits in Figure 5.14 shows the directionality from the non-isotropic scattering given by the scattering intensity equation (5.3). This is shown by the reflections for the Rayleigh scattered hits, located at the beamspot for $t_{res} = 290$ ns and at area around the injection point for $t_{res} = 390$ ns. This directionality is not present in the case for the re-emitted hits in Figure 5.13 because of the isotropic nature of re-emission.
Figure 5.9: PSUP hit map of \textbf{HitOpReemission} category events for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.

Figure 5.10: PSUP hit map of \textbf{HitOpRayleigh} category events for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.
Figure 5.11: Residual time vs. $\cos(\theta_{\text{wrf}})$ hit map of HitPMT category events for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.

Figure 5.12: Residual time vs. $\cos(\theta_{\text{wrf}})$ hit map of HitConc category events for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.
Figure 5.13: Residual time vs. $\cos(\theta_{\text{wrfp}})$ hit map of HitOpReemission category for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.

Figure 5.14: Residual time vs. $\cos(\theta_{\text{wrfp}})$ hit map of HitOpRayleigh category events for a pure liquid scintillator simulation of AMELLIE with light injection at node ID 73.
Chapter 6

Regions of Interest

By the classifications of simulation data presented in Chapter 5, a deeper understanding of the simulated detector output has been achieved. Applied to detector output from either RAT simulations or from real calibration data, the different features presented by graphical representations, such as in Figure 5.1 and Figure 5.4, can be understood with respect to the physical processes inside the detector.

In this chapter the classification categories will be further used to identify regions of interest in the residual time vs. $\cos(\theta_{\text{wrfp}})$ hit map. The purpose of these regions is to amplify the detected effects that occur when studying optical degradations. This will be achieved by selecting regions that are focusing on specific types of PMT hits while attempting to exclude others. These regions of interest can further be used to monitor the optical properties of the SNO+ detector by the AMELLIE calibration system.

6.1 Determining sections in residual time vs. $\cos(\theta_{\text{wrfp}})$

Based on the discussions in Chapter 5, the different types of PMT hits causing the different intensity peaks in the residual time vs. $\cos(\theta_{\text{wrfp}})$ hit map are known. From this, an initial set of sections in the residual time vs. $\cos(\theta_{\text{wrfp}})$ picture can be defined, attempting to isolate the different types of PMT hits. The initial sections are presented in Figure 6.1 with the numeric definitions and a short description presented in Table 6.1.

In order to be able to select the right regions of interest it is important to know the way optical degradations will be introduced in the simulations, and what effects can be expected. Optical degradation will be introduced by reducing the absorption length\(^1\) of the liquid scintillator mix, which is described in detail in Chapter 7. With a lower

\(^1\) Absorption length is the distance $\lambda$ into a material where the intensity of a beam will have dropped to $\frac{1}{e} \approx 63\%$. 
Figure 6.1: Graphical representation in the residual time vs. $\cos(\theta_{wrfp})$ hit map of the initial set of sections.

Table 6.1: Definitions of initial residual time vs. $\cos(\theta_{wrfp})$ sections.

<table>
<thead>
<tr>
<th>Section ID</th>
<th>$\cos(\theta_{wrfp})$</th>
<th>$t_{res}$</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beamspot</td>
<td>[-1.0, -0.93]</td>
<td>[240, 265]</td>
<td>Beamspot, mostly Hit category.</td>
</tr>
<tr>
<td>Directrefl</td>
<td>[0.95, 1.0]</td>
<td>[255, 285]</td>
<td>Reflections against near side of AV.</td>
</tr>
<tr>
<td>Beamspotrefl</td>
<td>[-1.0, -0.95]</td>
<td>[280, 300]</td>
<td>Reflections from beamspot against AV.</td>
</tr>
<tr>
<td>HitPMTdelrefl</td>
<td>[0.4, 0.7]</td>
<td>[360, 390]</td>
<td>Mostly reflected HitPMT category hits from far side of AV.</td>
</tr>
<tr>
<td>HitConcdelrefl</td>
<td>[0.9, 1.0]</td>
<td>[400, 420]</td>
<td>Mostly reflected HitConc category hits from far side of PSUP structure.</td>
</tr>
<tr>
<td>HitRaydelrefl</td>
<td>[0.9, 1.0]</td>
<td>[380, 400]</td>
<td>Mostly reflected HitOpRayleigh category hits from far side of AV.</td>
</tr>
<tr>
<td>DirectReemRay</td>
<td>[-0.8, 0.8]</td>
<td>[240, 280]</td>
<td>Early re-emitted and Rayleigh scattered.</td>
</tr>
</tbody>
</table>
absorption length, more of the fibre injected beam will be absorbed inside the AV, which will result in fewer PMT hits at the beamspot. Additionally, as a consequence of the increase of absorptions, more photons will be re-emitted from the liquid scintillator in the AV, causing a increase in PMT hits from re-emitted light.

Attempting to isolate these effect from the optical degradations, regions of interest where detected PMT hits decrease due to more absorption and where detected PMT hits increase due to more re-emission, will be selected. Both effects will be present across the whole residual time vs. \( \cos(\theta_{\text{wrfp}}) \) picture, but to different degrees. Taking this into account, the selected regions needs to maximise the influence of one of the effects, while at the same time minimise the influence of the other.

Of the initial sections, presented in Figure 6.1, the Beamspot section is selected for the study of the drop in overall hits due to an increase of absorptions. This is because the beamspot consists of most of the Hit category hits and the PMT hits within the beamspot is dominated by Hit category hits. In order to study the expected increase in re-emitted PMT hits the DirectReemRay region is selected, because it contains an high intensity of HitOpReemission category hits and very few Hit category hits. It is important to note that the DirectReemRay also includes an high intensity of HitOpRayleigh, which will affect the overall hit rate inside the section.

### 6.2 Efficiency and Purity in res. time vs. \( \cos(\theta_{\text{wrfp}}) \) sections

The boundaries of the Beamspot and DirectReemRay sections were initially defined based on a visual analysis of residual time vs. \( \cos(\theta_{\text{wrfp}}) \) hit maps of different hit categories in Chapter 5. In order to justify the definitions of the selected sections a quantitative analysis of the sections is needed, keeping in mind the purpose of the sections and what kind of degradation effects they focus on.

Attempting to maximise the presence of the specific hit PMT category in focus for the specific section, a measure is needed to compare different selections of boundaries for the section with this in mind. For this purpose, the Efficiency (6.1) and the Purity (6.2) of a specific PMT hit categories within a residual time vs. \( \cos(\theta_{\text{wrfp}}) \) subsection, is defined. **Efficiency** is the ratio of the specific category hits within the section to the total amount of the specific category hits in the detector. **Purity** is the ratio of the specific category hits within the section to the total hits overall (effectively HitOther category hits) within the section.
The Beamspot section is attempting to study the effects on the Hit category hits and the DirectReemRay section is attempting to study the effects on the HitOpReemission. To achieve this it is beneficial to maximise the amount of the specific category hits within the section, high Efficiency, as well as to maximise the amount of the PMT hits within the sections that are of the specific category, high Purity. For this purpose the figure of merit, called EffPur (6.3), is introduced. The EffPur value is the product of the Efficiency and the Purity of a specific hit category within a section.

\[
\text{EffPur} = \text{Efficiency} \cdot \text{Purity}
\] (6.3)

In Figure 6.2 and Figure 6.3 the EffPur values of the hit categories Hit, HitOpReemission and HitOpRayleigh are presented for the initial sections defined in Figure 6.1 and in Table 6.1. The figures show results from AMELLIE simulations for the pure scintillator phase and Te-loaded scintillator phase respectively. The pure scintillator phase simulation is initiated by the RAT macro in Code A.1 which is the same simulation that has been referred to in previous chapters. Both figures show that the Beamspot and DirectReemRay sections are the best sections to study the effect on the Hit category and on the HitOpReemission category. For the Beamspot section the EffPur value for the Hit category is about 0.86 for pure scintillator phase and about 0.78 for Te-loaded phase, while the EffPur values for the other categories are close to zero. On the other hand, for the DirectReemRay section the EffPur value for Hit category hits is about zero, but EffPur value for HitOpReemission and HitOpRayleigh category hits are notable.

Similar simulations have been done for other wavelengths, 403 nm, 419 nm, 451 nm, 470 nm, 488 nm and 511 nm, giving almost identical results for the EffPur values for the sections shown in Figure 6.2 and in Figure 6.3. An expectation to this was however observed for the Te-loaded scintillator simulations when using the shorter wavelengths, especially 403 nm but also 419 nm. For these two cases the EffPur value for Hit category hits in the Beamspot section was much lower than for the other cases. In addition to this, higher EffPur values for HitOpReemission category hits in the Directrefl and DirectReemRay sections was observed. In order to demonstrate this, the EffPur values in the case of 403 nm light in the Te-loaded scintillator phase are presented in Figure 6.4, Figure 6.5.
Figure 6.2: **EffPur** values for the hit categories Hit, HitOpReemission and HitOpRayleigh within the residual time vs. $\cos(\theta_{\text{wrfp}})$ sections defined in Table 6.1. Simulations of AMELLIE in the pure scintillator phase with light 434 nm wavelength.

Figure 6.3: **EffPur** values for the hit categories Hit, HitOpReemission and HitOpRayleigh within the residual time vs. $\cos(\theta_{\text{wrfp}})$ sections defined in Table 6.1. Simulations of AMELLIE in the Te-loaded scintillator phase with light 434 nm wavelength.
shows the PSUP hit map for 403 nm wavelength when used for the Te-loaded scinitllator phase. In this figure the largest concentration of hits is not in the beamspot but back at the injection point. This is due to much higher rates of absorption and re-emission causing large attenuation of the fibre emitted pulse. The wavelengths 403 nm and 419 nm are included in the degradation study, but it is important to be aware of the difference in the output observed for these two cases.

It is important to note that the EffPur values does not indicate the absolute number of hits in the sections. Because of this each EffPur value have to be evaluate in the context of the size and position of the sections as well as the evaluated hit category. For example, as the Hit category is mainly concentrated in the beamspot all section that does not include the beamspot will have a low Efficiency value for the Hit category which will downscale the EffPur value in cases where the Purity of the Hit category is higher, such as in the HitPMTdelrefl and HitConcdelrefl sections.

6.3 Optimisation and stability of the Beamspot section

The measure by which the merits of the selected sections can be evaluate is defined. The EffPur value can now be used to optimise the definitions of the sections and evaluate the stability of the section. The definition of the Beamspot section, see Table 6.1, will be evaluated first. For this section the goal is to maximise the EffPur value for the Hit category.

Figure 6.6 and Figure 6.7 presents the results of the optimisation of the section definition. The optimisation process, that are presented by the figures, use the boundary values as given by the original definition as fixed values, while adjusting one of the sides and calculating the EffPur value for the adjusted section. In the case of the Beamspot no adjusting is done on the lower bound residual time of the section, because the centre of the beamspot is located at \( \cos(\theta_{wrfp}) = -1 \).

The result of the optimisation in the case of the Beamspot section is that the EffPur peak values are obtained by the original section definition of the Beamspot, given in table 6.1. Additionally, with regards to the stability on the EffPur values from Beamspot section, the EffPur value is more or less unchanged if we Beamspot section is extendive and negative residual time from the original definition. Also, with a variation of about 0.1 on the original definition of the upper bound of the \( \cos(\theta_{wrfp}) \) the EffPur value changes very little. For an upper boundary on \( \cos(\theta_{wrfp}) \) within the range \([-0.95, -0.90]\] the EffPur value is relatively stable.
Figure 6.4: EffPur values for the hit categories Hit, HitOpReemission and HitOpRayleigh within the residual time vs. $\cos(\theta_{wrfp})$ sections defined in Table 6.1. Simulations of AMELLIE in the Te-loaded scintillator phase with light 403 nm wavelength.

Figure 6.5: PSUP hit map of HitOther category events for a Te-loaded liquid scintillator simulation of AMELLIE with light injection at node ID 73. Wavelength used is 403 nm.
Figure 6.6: EffPur values for variations on the $\cos(\theta_{wrfp})$ upper bound for the Beamspot section for Hit category hits.

(a) Variations on the residual time lower bound. (b) Variations on the residual time upper bound.

Figure 6.7: EffPur for variations on the residual time for the Beamspot section for Hit category hits.
6.4 Optimisation and stability of DirectReemRay section

In the case of the DirectReemRay section, the goal of the optimisation is to maximise the EffPur value for the HitOpReemission category. The results of the optimisation are included in Figure 6.8 and in Figure 6.9. As opposed to the case of the Beamspot section, the original definition of the DirectReemRay section does not correspond to the peak values of EffPur for HitOpReemission category hits. Rather, it appears as if the ranges $\cos(\theta_{wrfp}) \in [-0.94, 0.98]$ and $t_{res} \in [258, 365]$ are the section definition that results in the peak value of EffPur in the case of the DirectReemRay section.

These new section definitions are used to redefine an optimised section of the original DirectReemRay section, which will be called the DirectReemRayO section. The new definition for DirectReemRayO, which is shown graphically in Figure 6.12, has increased in size and moved position compared to the original DirectReemRay section. In order to justify this new definition the optimisation procedure is performed again for new definition of the section. The results are included in Figure 6.10 and in Figure 6.11. These plots confirm that the peak value of EffPur is obtained by the new and optimised section definition for the DirectReemRay section. The stability of the DirectReemRayO section can be inferred from Figure 6.10 and Figure 6.11.

6.5 Final definitions of Beamspot and DirectReemRay

The optimisation procedure have been performed for both the Beamspot and DirectReemRay sections, which is the two section that will be the main focus when studying the optical degradations. An optimised and redefined section, DirectReemRayO, was defined based on the DirectReemRay section. The final definitions of these sections, are included in Table 6.2 where the original definition of the DirectReemRay section is kept as a reference. Further, these final section definitions can also be seen graphically in the residual time vs. $\cos(\theta_{wrfp})$ hit map on Figure 6.12.

Additionally, in Figure 6.13 the new EffPur values for the hit categories Hit, HitOpReemission and HitOpRayleigh are presented for the final section definitions. This is to show again how the different hit categories are present in the different sections, but also to show what is gained with respect to the DirectReemRay section by doing the optimisation described above.

The optimisations process in Section 6.3 and Section 6.4 that obtained the final section defintions in Table 6.2 are done for the pure scintillator phase simulation with the 434 nm
(a) Variations on the $\cos(\theta_{wrfp})$ lower bound. (b) Variations on the $\cos(\theta_{wrfp})$ upper bound.

Figure 6.8: $\text{EffPur}$ values for variations on the $\cos(\theta_{wrfp})$ for the DirectReemRay section for HitOpReemission category hits.

(a) Variations on the residual time lower bound. (b) Variations on the residual time upper bound.

Figure 6.9: $\text{EffPur}$ for variations on the residual time for the Beamspot section for HitOpReemission category hits.
(a) Variations on the \( \cos(\theta_{wrfp}) \) lower bound.  
(b) Variations on the \( \cos(\theta_{wrfp}) \) upper bound.

Figure 6.10: \textbf{EffPur} values for variations on the \( \cos(\theta_{wrfp}) \) for the \textit{DirectReemRayO} section for \textit{HitOpReemission} category hits.

(a) Variations on the residual time lower bound. (b) Variations on the residual time upper bound.

Figure 6.11: \textbf{EffPur} for variations on the residual time for the \textit{DirectReemRayO} section for \textit{HitOpReemission} category hits.
wavelength. This section definitions is not necessarily the best definition for the other wavelengths, or in the case of the Te-loaded scintillator phase. Because of this the same optimisation has been performed for all wavelengths for both the Te-loaded scintillator phase and for the pure scintillator phase. The resulting section definitions for the Beamspot and the DirectReemRayO, as well as the corresponding EffPur value is given in Table 6.3 and in Table 6.4 respectively.

Table 6.2: Definitions of final residual time vs. $\cos(\theta_{wrfp})$ sections for the LED434 wavelength distribution for the pure scintillator phase.

<table>
<thead>
<tr>
<th>Section ID</th>
<th>$\cos(\theta_{wrfp})$</th>
<th>$t_{res}$</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beamspot</td>
<td>[-1.0, -0.93]</td>
<td>[240, 265]</td>
<td>Final section definition.</td>
</tr>
<tr>
<td>DirectReemRay</td>
<td>[-0.8, 0.8]</td>
<td>[240, 280]</td>
<td>Original section definition.</td>
</tr>
<tr>
<td>DirectReemRayO</td>
<td>[-0.94, 0.98]</td>
<td>[258, 365]</td>
<td>Redefined and final section.</td>
</tr>
</tbody>
</table>
Figure 6.12: Final sections in Residual time vs. $\cos(\theta_{wrfp})$ hit map, Beamspot, DirectReemRay and the optimised and redefined DirectReemRayO.

Figure 6.13: EffPur values for the hit categories Hit, HitOpReemission and HitOpRayleigh within the final residual time vs. $\cos(\theta_{wrfp})$ sections defined in Table 6.2. Simulations of AMELLIE in the pure scintillator phase with light 434 nm wavelength.
Table 6.3: Definitions of the *Beamspot* section for all wavelengths with corresponding *EffPur* values for *Hit* category hits.

<table>
<thead>
<tr>
<th>Wavelength</th>
<th>Pure scint.:</th>
<th>Te-loaded:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>cos((θ_{wrfp}))</strong></td>
<td><strong>(t_{res})</strong></td>
</tr>
<tr>
<td>403 nm</td>
<td>[-1.0, -0.93]</td>
<td>[240, 265]</td>
</tr>
<tr>
<td>419 nm</td>
<td>[-1.0, -0.93]</td>
<td>[240, 265]</td>
</tr>
<tr>
<td>434 nm</td>
<td>[-1.0, -0.93]</td>
<td>[240, 265]</td>
</tr>
<tr>
<td>451 nm</td>
<td>[-1.0, -0.93]</td>
<td>[240, 265]</td>
</tr>
<tr>
<td>470 nm</td>
<td>[-1.0, -0.93]</td>
<td>[240, 270]</td>
</tr>
<tr>
<td>488 nm</td>
<td>[-1.0, -0.92]</td>
<td>[240, 270]</td>
</tr>
<tr>
<td>511 nm</td>
<td>[-1.0, -0.92]</td>
<td>[240, 270]</td>
</tr>
</tbody>
</table>

Table 6.4: Definitions of the *DirectReemRayO* section for all wavelengths with corresponding *EffPur* values for *HitOpReemission* category hits.

<table>
<thead>
<tr>
<th>Wavelength</th>
<th>Pure scint.:</th>
<th>Te-loaded:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td><strong>cos((θ_{wrfp}))</strong></td>
<td><strong>(t_{res})</strong></td>
</tr>
<tr>
<td>403 nm</td>
<td>[-0.96, 0.99]</td>
<td>[258, 365]</td>
</tr>
<tr>
<td>419 nm</td>
<td>[-0.95, 0.98]</td>
<td>[258, 365]</td>
</tr>
<tr>
<td>434 nm</td>
<td>[-0.94, 0.98]</td>
<td>[258, 365]</td>
</tr>
<tr>
<td>451 nm</td>
<td>[-0.94, 0.98]</td>
<td>[258, 364]</td>
</tr>
<tr>
<td>470 nm</td>
<td>[-0.94, 0.98]</td>
<td>[258, 360]</td>
</tr>
<tr>
<td>488 nm</td>
<td>[-0.94, 0.99]</td>
<td>[258, 360]</td>
</tr>
<tr>
<td>511 nm</td>
<td>[-0.93, 0.98]</td>
<td>[256, 360]</td>
</tr>
</tbody>
</table>
Chapter 7

Optical degradation

7.1 Introducing optical degradation into the simulations

The optical properties of the scintillator material used in RAT simulations are loaded from a database file. This database file contain various optical properties of the material, like the refractive indices, absorption lengths and Rayleigh scattering lengths for different wavelengths. The way optical degradations are introduce in this study is in the form of reductions of to the values of the absorption lengths for the LAB material in the liquid scintillator. For a overview of the different materials and their absorption lengths we have included them as a function of wavelengths in Figure 7.1. When simulations are performed for the pure liquid scintillator phase the scintillator mix only consists of LAB (blue) and PPO (red), while for the Te-loaded phase Te (green) and a wavelength shifter, in these simulations bisMSB (orange) is added.

The option in the RAT simulations that can be used to degrade the absorption lengths is the ABSLENGTH_SCALING parameter. This parameter scales the absorption length spectrum by the factor

\[
\frac{1}{\text{ABSLENGTH_SCALING}}
\]

In order to degrade the absorption length spectrum of a specific material by 10% we need to set the ABSLENGTH_SCALING for this material to 1.111. This corresponds to a scaling-factor of \(1/1.111 \approx 0.9\).

7.2 Simulations and results with optical degradation

In this section results of simulations where various optical degradations are applied will be presented and discussed. The analysis will be done by using the regions of interest defined
Figure 7.1: Absorption lengths for components in the liquid scintillator mix for the SNO+ experiment. For the pure scintillator phase the mix will consist only of LAB and PPO, while for the Te-loaded phase it will also consist of Te and bisMSB.

A set of simulations have been performed, where a range different simulations parameters have been used. The purpose of the different simulations is to demonstrate how the simulation parameters affect the results of the degradation study, as well as to compare the the different parameters. Bellow, the different simulation parameters used for the degradation study are listed. The number in the parenthesis after each parameter indicates the number of options for this parameter. In parenthesis for the listed options for each parameter is the name of what the option as called in the RAT macro file.

**Wavelength distributions (7)** 403 nm (LED403simple), 419 nm (LED419simple), 434 nm (LED434simple), 451 nm (LED451simple), 470 nm (LED470simple), 488 nm (LED488simple), 511 nm (LED511simple)

**Scintillator material (2)** Pure scintillator (snoplus.geo), Te-loaded scintillator (snoplus_te.geo)

**Fibre beam intensity (3)** 1000, 1500, 3000

**Degradations on LAB (3)** 0 (1.0), 10% ($\frac{4}{1.11} \approx 0.9$), 20% ($\frac{4}{1.25} = 0.8$)
The simulations has been performed by the use of a batch job script, an example is given in Code A.4. The example performes simulations for all the different fibre beam intensities and different degradations with the detector in the pure liquid scintillator phase and 434 nm wavelength on the injected light. This batch job script utilise and modify a base RAT macro file, given in Code A.5.

In the following sections the effects of the different degradations on each of the variables as well as for our designated regions of interest wil be presented and discussed. This will be done by viewing the effects of degradation in the form of bar diagrams with the various parameters along the x-axis and the “Change of PMT hits” along the y-axis, unless otherwise specified.

When not otherwise specified, the “Change of PMT hits” in the bar diagrams indicates the change of the HitOther category PMT hits within the specified section. The “Change of PMT hits” is the ratio of the number of hits in the simulation where degradations are included with respect to a identical simulation without any degradation on the liquid scintillator mix. The ratio is subtract by 1 before it is inserted into the bar diagram. This is done in order for the bar diagram to indicate the change, with positive values indicating an increase in the HitOther category PMT hits and negative values indicating a decrease. The reason why focus is on the change of the HitOther PMT hit category is, as mentioned before, because this is the simulated detector output that corresponds to the detector output from a real life calibration measurement.

The errors included in the bar diagrams are initially calculated from the number of hits $N$ counted within a section. Assuming that the hits follow Poisson statistics we get an uncertainty of $\sqrt{N}$ on the counted value. These counting uncertainties are then used to calculate the uncertainty on the change in hits, by using standard uncertainty propagation formulas.

It is important to mentioned here that as the bar diagrams presents the change in the HitOther category we are neglecting the detector noise in the simulations, that are classified in the Noise category. Detector noise, as well as background noise, will play a role in the real life calibration measurements, so it is important to be aware that these are not included in the following results.

### 7.2.1 Wavelength distributions

This section will present how injected light of different wavelength distributions are affected in both the pure liquid scintillator and the Te-loaded scintillator, when the LAB absorption
length is degraded by 10%. In Figure 7.2 the “Change of PMT hits” are presented for inside the Beamspot section. In Figure 7.3 the same is presented for the DirectReemRayO section.

For the diagrams for the Beamspot section, the PMT hits inside the section is decreasing for both for all wavelengths. In the case of the pure scintillator simulations, in Figure 7.2a it appears that the decrease of PMT hits inside the Beamspot section follows a pattern. The reduction in PMT hits is weaker for longer wavelengths. This pattern is similar to the pattern of the absorption length of the LAB material, given in Figure 7.1. The absorption length is increasing for longer wavelengths from 400 nm to 500 nm. However, for the 511 nm wavelength the absorption length decrease to about the same level as it was for about 460 nm, but there is no sign of that in the bar diagram. There is some indications of this pattern in the diagram for the case of the Te-loaded scintillator phase, in Figure 7.2b, but especially for low wavelengths the uncertainty is too high to discern any pattern.

Next, for the diagrams of the DirectReemRayO section, at least for the pure scintillator case in Figure 7.3a a weak increase in hits for all wavelengths is present. The results for the Te-loaded case, in Figure 7.3b only consists of small changes and large uncertainties for all wavelengths. To understand why the decrease in signal hits inside the Beamspot is more distinct than the increase inside the DirectReemRayO section we need to look back at the EffPur results for the sections in Figure 6.13 (page 65).

From this graph it can be concluded that, since the EffPur for the Hit category is large for the Beamspot section, the overall hits inside the section is largely dominated of Hit category hits. On the other hand, for the DirectReemRayO section the EffPur for the HitOpReemission is not dominant and lower than for the HitOpRayleigh category. This indicates that the effects of degradations inside the DirectReemRayO section consists of the effect on both the re-emitted and the Rayleigh scattered light. The weak change within the DirectReemRayO section is because the decrease of re-emitted PMT hits are concealed by a increase of the more numerous Rayleigh scattered PMT hits.

7.2.2 Fibre pulse intensities

This section will present how the different beam intensities from the injection fibres are affected by the degradation. In Figure 7.4 this is presented for inside the Beamspot section for both the pure scintillator phase and the Te-loaded phase. The same for inside the DirectReemRayO section is included in Figure 7.5. The 434 nm wavelength distribution
Figure 7.2: Change in detected PMT hits for different wavelengths inside the Beamspot section. Degradation of the LAB absorption length by 10%.

(a) Pure scintillator phase  
(b) Te-loaded phase

Figure 7.3: Change in detected PMT hits for different wavelengths inside the Beamspot section. Degradation of the LAB absorption length by 10%.

(a) Pure scintillator phase  
(b) Te-loaded phase
is chosen for the simulations with different the beam intensities.

Most of the results for different intensities are within the uncertainty of each other, which makes it difficult to say anything about the effect of the different intensities. Higher intensity basically means more photons in the fibre emitted pulse. If one takes into account multi PE hits on in the PMTs, two photons hitting a PMT with very small temporal difference and are registered as one hit by the PMT, a difference with higher intensity, where this happens more frequently, should be present. We can conclude from our diagrams that in the case of this effect, with the simulations of the beam intensities 1000, 1500 and 3000, there are no clear detectable effect within the uncertainties on the bar diagrams. Further simulations we will be using the intensity of 3000 for the fibre beams.

7.2.3 Degrees of degradation

The next simulation parameter to study is the different degrees of degradation, and how they effect the PMT hits inside the Beamspot and the DirectReemRayO sections. The degrees of degradation that will be studied is degradations of the LAB absorption lengths of 10%, which is the same as what we have used until now, and of 20%. Figure 7.6 contains the results from simulations of these different degrees of degradation when looking at the Beamspot section for both the pure scintillator phase and the Te-loaded phase. Figure 7.7 contains the same corresponding results but for inside the DirectReemRayO section.

First, there is the results for the Beamspot section, with the pure scintillator case in Figure 7.6a and the Te-loaded case in Figure 7.6b. For the pure scintillator case with 10% degradation on the LAB the change of HitOther category PMT hits within the Beamspot section is about a 1.6% decrease. And with a 20% degradation this turns into about a 3.3% decrease on the detected hits, a doubling of the decrease for 10% degradation. On the other hand, for the Te-loaded scintillator 10% degradation gives about a 1.1% decrease, while 20% degradation gives about a 2.8% decrease.

The effect of degradations on the absorption lengths of the LAB is weaker for the Te-loaded scintillator then for the pure scintillator. However, when increasing the degradation from 10% to 20% the effects in the case of the Te-loaded scintillator change by a factor of 2.5 as opposed to the doubling for the pure scintillator. This is because of the fact that in the case of the Te-loaded scintillator the Tellurium and the wavelength shifter which has absorption lengths that are lower than for the LAB. Since the scintillator mix mostly consists of LAB this effect is small.
Figure 7.4: Change in detected PMT hits for different fibre beam intensities inside the Beamspot section. Degradation of the LAB absorption length by 10%.

Figure 7.5: Change in detected PMT hits for different fibre beam intensities inside the DirectReemRayO section. Degradation of the LAB absorption length by 10%.
Secondly, there is the results from the *DirectReemRayO* section. In the case of the pure liquid scintillator, in Figure 7.7a, a small increase of about 0.8% is present for 10% degradation on the LAB. This increase to about a 1.7% increase with 20% degradation. For the Te-loaded scintillator, in Figure 7.7b, the change is even weaker and the change from both 10% and 20% degradation is within each other uncertainties, although a small increase is visible.

### 7.3 Regions of interest

A selection of simulation parameters have been studied with respect to the effects of degradations on the LAB absorption lengths. The parameters that have been studied are: the wavelength distribution, the fibre beam intensity and the degree of degradation. This section will go deeper into the regions of interest that was defined in Chapter 6, analyse their merits and compare them to see the combined result from looking at various regions at the same time.

In the discussion on the different wavelength distributions in Section 7.2.1, it was mentioned that the expected decrease of the hits in the *DirectReemRayO* section is not that clear, because of an increase in re-emitted light. This is because the *HitOther* category hits inside the section also consists of a lot of *HitOpRayleigh* category hits in addition to the *HitOpReemission* category hits, and also a few *Hit* category hits. In most of the cases the *HitOpRayleigh* category hits outnumber the *HitOpReemission* category hits around 4 to 7 times. This effect can be studied by going further into the contents of the sections by presenting the change of the *HitOpReemission* category hits and the *HitOpRayleigh* category hits along with the *HitOther* category hits.

In Figure 7.8 the degradation results are presented for the look into this we have can pure scintillator case. To clarify the bin labels in the bar diagram, the start of the bin label is the abbreviate of the section, BS for the *Beamspot* section and DRRO for the *DirectReemRayO* section. Following this is the PMT hit category. First of, the results for the *Beamspot* section shown an increase in the re-emitted light and a decrease in the Rayleigh scattered light for both degrees of degradation. Also, the large error bars compared to the *HitOther* category is due to the small amount of *HitOpReemission* and *HitOpRayleigh* hits inside the Beamspot, as expected from the *EffPur* value of the *Beamspot* section. The consequence of this is that the change in these two categories plays a small part in the overall change in this section, as intended for the *Beamspot* section.

Next, for the *DirectReemRayO* section results the uncertainty of the *HitOpReemis-
Figure 7.6: Change in detected PMT hits for different degrees of degradation inside the Beamspot section.

Figure 7.7: Change in detected PMT hits for different degrees of degradation inside the DirectReemRayO section.
sion and HitOpRayleigh hits are less than in the Beamspot section, indicating better statistics for these hit types inside the section. Further, the considerable change in the re-emitted hits occurs, with about 8% increase for 10% degradation and about 17% increase for 20% degradation. This change is the change that was the initially purpose of the DirectReemRayO section to uncover in the HitOther category. However, the change of the HitOther category is much weaker in the bar diagram, for both 10% and 20% degradation. This is because of the decrease of the much more numerous HitOpRayleigh hits within the DirectReemRayO section. This change is small, as seen in the diagrams, but because of more hits counterbalance the increase in re-emitted hits.

Looking at the same case for the Te-loaded scintillator case in Figure 7.9 a similar picture that has been described for the pure scintillator case can be seen.

Next, the various regions of interest as defined in Table 6.2 will be compared. Changes both within these sections as well as outside the sections are studied, because as an increase of hits within the Beamspot section is expected, it could be interesting to see if that results in an overall decrease of hits outside the Beamspot section.

Also, four addition sections have been added, which will be called ResTimeCut sections. The idea of these sections is to look outside the Beamspot section, but put an upper bound on the residual time. Full definitions are included in Table 7.1 for the ResTimeCut sections. The reason for adding these sections is to look at a more broader way, only restrict the time parameter, to view the hits than the optimised sections defined in Chapter 6.

Table 7.1: Definitions of ResTimeCut sections in the Residual time vs. $\cos(\theta_{wrfp})$ picture.

<table>
<thead>
<tr>
<th>Section ID</th>
<th>$\cos(\theta_{wrfp})$</th>
<th>$t_{res}$</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ResTimeCut1</td>
<td>[-1.0, 1.0]</td>
<td>[210, 300]</td>
<td>Excluding Beamspot section.</td>
</tr>
<tr>
<td>ResTimeCut2</td>
<td>[-1.0, 1.0]</td>
<td>[210, 330]</td>
<td>Excluding Beamspot section.</td>
</tr>
<tr>
<td>ResTimeCut3</td>
<td>[-1.0, 1.0]</td>
<td>[210, 380]</td>
<td>Excluding Beamspot section.</td>
</tr>
<tr>
<td>ResTimeCut4</td>
<td>[-1.0, 1.0]</td>
<td>[210, 420]</td>
<td>Excluding Beamspot section.</td>
</tr>
</tbody>
</table>

The sections where a decrease in hits is expected is presented first. These are the Beamspot section, but also, the sections outside the ResTimeCuts sections, which means all hit events after the given residual time cut, as well as outside of the DirectReemRayO section, excluding the contents of the Beamspot. The results in the case of 10% and 20% degradation for the pure scintillator care included in Figure 7.11.

This figure shows the decrease in the Beamspot section, as previously studied. Then
Figure 7.8: Change in detected PMT hits for different hit PMT categories in *Beamspot* and *DirectReemRayO* sections for the pure scintillator phase.

(a) 10% degradation  
(b) 20% degradation

Figure 7.9: Change in detected PMT hits for different hit PMT categories in *Beamspot* and *DirectReemRayO* sections for the Te-loaded phase.

(a) 10% degradation  
(b) 20% degradation

Figure 7.10: Change in detected PMT hits for different res. time vs. $\cos(\theta_{\text{wrfp}})$ sections, where we expect a decrease in hits, for the pure scintillator phase.

(a) 10% degradation  
(b) 20% degradation
there is the results for outside the ResTimeCut regions. Here, a larger decrease is achieved for the higher the residual time cut of is, but also by for higher residual tim cuts the statistics gets poorer because of the low hit rates for the reabove thee high residual time cuts. The area outside the DirectReemRayO section, excluding the beamspot hits, get about a 0.9% decrease with 10% degradation on the LAB absorption lengths, and about a 2.4% decrease with 20% degradation. These values, and the error bars, for outside the DirectReemRayO section are similar to the corresponding values for above the ResTime-Cut2 section. The regions outside these two sections share a lot of the same data, and the observed decrease is because of the decrease of the large amount of HitOpRayleigh category hits in these regions, as was seen in Figure 7.8 and Figure 7.9.

Secondly, by looking at the sections where an increase in the hits are expected, which is be mainly due to an increase in re-emitted light. The sections to be presented are the area everything outside of the Beamspot section, the areas inside the DirectReemRay and the DirectReemRayO sections, and the areas inside the four ResTimeCut sections, with the Beamspot hits excluded. The results in the case of 10% and 20% degradation for the pure scintillator care included in Figure 7.10.

The first thing to point out for both degrees of degradation is that there is little to gain from looking at the region outside the Beamspot section. The reason for this small change is due to the mix of different categories in the area outside the Beamspot. This seem to also apply to some degree for the for the other sections, even though a minor increase of around 0.30% is seen, when looking at 10% degradation, in Figure 7.11a. These differences are a somewhat larger for 20% degradation on the LAB, Figure 7.11b, with an about 0.47% increase of hits.

7.4 Degradation measure

In the previous sections how its was studied how degradations on the LAB absorption lengths have effected our simulations differently with respect to various simulation parameters and when looking at different \( \cos(\theta_{\text{wrfp}}) \) regions. From this study it can be concluded that the changes observed, when looking at the designated regions of interest, Table 6.2, as well as other derived regions, is in most cases weak and sometimes inconclusive because of weak change and low statistics. In this section a measure that can improve the measurements of optical degradations will be defined.

The way we will approach this is by first point out that the changes that is observeed in sections such as the Beamspot, DirectReemRayO and outside the DirectReemRayO, ex-
cluding beamspot hits, not directly depend on each other. This is because these specific sections does not intersect each other, and thereby does not share any PMT hit events. Using the fact that the total PMT hits (\textit{HitOther} category) is decreasing within the \textit{Beamspot} section and outside the \textit{DirectReemRayO} section, and increasing in the \textit{DirectReemRayO} section, the following measure is designed (7.1).

\[
\text{DegradationMeasure} = \frac{\text{Beamspot} \times \text{OutsideDirectReemRayO}}{\text{DirectReemRayO}} \tag{7.1}
\]

In the equation for the \textit{DegradationMeasure} (7.1) the ratio of the number of hits with degradation against the number of hits without degradation for the \textit{Beamspot} and the \textit{OutsideDirectReemRayO} sections are multiplied, then this is divided by the corresponding ratio for the \textit{DirectReemRayO} section.

The reason why these specific sections has been chosen instead of some of the others of the sections studied in Figure 7.11 and Figure 7.10 is mainly because of the low uncertainty on the results from these sections. Also, these are the sections for which we performed the optimisation when defining them in Chapter 6 giving us a better understanding of what they contain and the stability on the definitions.

The results obtained for the \textit{DegradationMeasure} in the case of a pure scintillator phase simulation is given in Figure 7.12. These figures presents the results for the different wavelength distributions and for both the 10\% (Figure 7.12a) and the 20\% (Figure 7.12b) degradation on the LAB absorption lengths. First of, pattern mentioned when talking about the results in Figure 7.2 (page 71) can be recognised.

The corresponding results of the \textit{DegradationMeasure} for the Te-loaded phase is presented in Figure 7.13. Because of the large uncertainties, it is still difficult in the case of the Te-loaded scintillator to see the difference between the wavelength distributions. On the other hand, with the introduction of the \textit{DegradationMeasure} changes are clearer for the same cases where we earlier obtained inconclusive change because of small changes and large uncertainties.

The numeric results for the \textit{DegradationMeasure} for the pure scintillator phase, as included in Figure 7.12 are presented in Table 7.2. The same for the Te-loaded phase, as included in Figure 7.13 is presented in Table 7.3. The regions of interest used for both the pure scintillator phase and the Te-loaded phase are fram Table 6.3 and Table 6.4. The values for the \textit{DegradationMeasure} in these tables is the directly calculated values from the section ratios as described by (7.1). For the values in the corresponding figures we have subtracted the calculated values by 1.
Figure 7.11: Change in detected PMT hits for different res. time vs. $\cos(\theta_{wrfp})$ sections, where we expect an increase in hits, for the pure scintillator phase.

Figure 7.12: Degradation Measure for different wavelength distributions for the pure scintillator phase.

Figure 7.13: Degradation Measure for different wavelength distributions for the Te-loaded phase.
Table 7.2: Numeric results of the DegradationMeasure for the pure scintillator phase.

<table>
<thead>
<tr>
<th>Wavelength dist.</th>
<th>DegMeasure$_{0.9}$</th>
<th>$\sigma_{0.9}$</th>
<th>DegMeasure$_{0.8}$</th>
<th>$\sigma_{0.8}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LED403simple</td>
<td>0.9467</td>
<td>0.0017</td>
<td>0.8854</td>
<td>0.0016</td>
</tr>
<tr>
<td>LED419simple</td>
<td>0.9621</td>
<td>0.0016</td>
<td>0.9159</td>
<td>0.0015</td>
</tr>
<tr>
<td>LED434simple</td>
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<td>0.0016</td>
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<td>0.0017</td>
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<tr>
<td>LED470simple</td>
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<td>0.0018</td>
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<td>0.0018</td>
</tr>
<tr>
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<td>0.0021</td>
<td>0.9793</td>
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<td>LED511simple</td>
<td>0.9745</td>
<td>0.0026</td>
<td>0.9538</td>
<td>0.0025</td>
</tr>
</tbody>
</table>

Table 7.3: Numeric results of the DegradationMeasure for the Te-loaded scintillator phase.

<table>
<thead>
<tr>
<th>Wavelength dist.</th>
<th>DegMeasure$_{0.9}$</th>
<th>$\sigma_{0.9}$</th>
<th>DegMeasure$_{0.8}$</th>
<th>$\sigma_{0.8}$</th>
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<tbody>
<tr>
<td>LED403simple</td>
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<td>0.009</td>
</tr>
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<td>0.9609</td>
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<td>0.0021</td>
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<tr>
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<td>0.9745</td>
<td>0.0026</td>
<td>0.9538</td>
<td>0.0025</td>
</tr>
</tbody>
</table>
Chapter 8

Conclusion

Detailed simulations of optical degradation of the liquid scintillator material inside the SNO+ experiment have been performed. The simulations emulate the optical calibration system, AMELLIE, which will be used to monitor the optical properties of the detector. Optical degradations are introduced into the simulations by reducing the absorption length of the LAB scintillator material in the detector.

Based on an in-depth study of the output from the performed simulations, a method to determine and optimise sections in the residual time vs. \( \cos(\theta_{\text{wrfp}}) \) picture (time and position of detected events) has been developed and used to determine regions of interest for the degradation study. These regions of interest, specifically the Beamspot and DirectReemRayO sections, have been used to analyse the different simulations with the aim of determining the degradations. By using the regions of interest, it has been shown how the detectable effects of the optical degradation can be amplified by combining changes of PMT hits in various sections.

This resulted in definition of the **DegredationMeasure** (7.1), which combines the changes cause by degradations in the Beamspot section, the DirectReemRayO section and the area outside the DirectReemRayO section. Applying the **DegredationMeasure** to the simulations of different wavelength distributions, in the case of the pure scintillator phase and the Te-loaded phase, resulted in the measures of optical degradation given in Table 7.2 and Table 7.3. The relevance of these values is that they are based on the same detected signal that could be measured by the AMELLIE calibration system.

The simulation data for the different detector phases and the different wavelength distributions were similar, except for short wavelengths, 403 nm and 419 nm, in the case of the Te-loaded scintillator phase. This anomaly is exemplified by Figure 6.4 and Figure 6.5.
It is important to mention that in this study the effect of multi PE hits in the simulation was not taken into account, nor was any convincing hints of multi PE hits present in the analysed data. However, this is something that is needed for further improvements of the degradation analysis.

Also, the Te-loaded mix (Te + bisMSB) used for the simulation is not the same as the one that will be used in the actual experiment, because of continued development. This is important to be aware of when comparing real calibration measurement from AMELLIE with these results.

In addition to taking into account multi PE hits and perform to simulations for a different Te-loaded scintillator mix, other further work includes making more simulations. The simulations could include different and more complex ways of introducing optical degradation, as well as increasing the statistic of the simulations. Also, more work on the regions of interest and the DegradationMeasure could be done in order to improve their merits.
Acknowledgements

First, I would like to thank my project supervisor and academic advisor at the University of Sussex, Lisa Falk. The many hours of meetings, discussion and e-mail exchanges has been essential for the progress of this project, as well as all the feedback along the way, which I am very grateful for. Also, I want to thank the people of the SNO+ group at Sussex: Ed, Simon, Mark, James and Lisa. It was nice to be included as a part of the research group.

Last but not least, I want to thank Hannah K. Lunde, my girlfriend, who has supported me through the project work and helped out with the proofreading of this report.
Bibliography


Appendix A

Code

If not stated otherwise then the code is written by the author.

Code A.1: AMELLIE_MCEV_Snoplus_LED434simple_abslengthscale_intensity3000_1_00.mac

```rat
# Brief: Simulate AMELLIE events (for details see below)
#
# This macro simulates AMELLIE events in the configuration
# FAann-DD_NN
# FAann identifies the fibre
# DD identifies the fibre slot on the SMELLIE/AMELLIE mounting plate
# (can be changed, for cross-checking the installation against data)
# NN is the no of simulated events
#
# Speed up rat initialisation time
/rat/physics_list/OmitMuonicProcesses true
/rat/physics_list/OmitHadronicProcesses true

# Simulate external async (mask 32768) trigger
# This trigger identifies ELLIE events
/rat/db/set DAQ_RUN_LEVEL trigger_mask 32768
/rat/db/set DAQ_RUN_LEVEL trigger_enable 35967

# Define the detector geometry for the simulation
/rat/db/set DETECTOR geo_file "geo/snoplus.geo"

# Edit optics, done by script
/rat/db/set OPTICS[labppo_scintillator] ABSLENGTH_SCALING [ 1.0, 1.0, ],

# Store all tracks
/rat/tracking/store full

# Select a fibre
# Options: FA089, FA189, FA073, FA173, FA050, FA150, FB012
# Also: FAx089−00, FAx089−10, FAx089−20; and similarly for the others
/rat/db/set ELLIE fibre_id "FA092"

# Set the number of photons per beam
# For fibre FA089 aiming for mean 343.5, rms 17.08
# Intensity 13522 gives nhits with a mean of 339.9, rms 13.43
/rat/db/set ELLIE intensity 3000
/rat/db/set ELLIE pulse_mode "poisson"

# Set the wavelength, timing and angular distributions
```

# Brief: Simulate AMELLIE events (for details see below)
# This macro simulates AMELLIE events in the configuration
# FAann-DD_NN
# FAann identifies the fibre
# DD identifies the fibre slot on the SMELLIE/AMELLIE mounting plate
# (can be changed, for cross-checking the installation against data)
# NN is the no of simulated events
#
# Speed up rat initialisation time
/rat/physics_list/OmitMuonicProcesses true
/rat/physics_list/OmitHadronicProcesses true

# Simulate external async (mask 32768) trigger
# This trigger identifies ELLIE events
/rat/db/set DAQ_RUN_LEVEL trigger_mask 32768
/rat/db/set DAQ_RUN_LEVEL trigger_enable 35967

# Define the detector geometry for the simulation
/rat/db/set DETECTOR geo_file "geo/snoplus.geo"

# Edit optics, done by script
/rat/db/set OPTICS[labppo_scintillator] ABSLENGTH_SCALING [ 1.0, 1.0, ],

# Store all tracks
/rat/tracking/store full

# Select a fibre
# Options: FA089, FA189, FA073, FA173, FA050, FA150, FB012
# Also: FAx089−00, FAx089−10, FAx089−20; and similarly for the others
/rat/db/set ELLIE fibre_id "FA092"

# Set the number of photons per beam
# For fibre FA089 aiming for mean 343.5, rms 17.08
# Intensity 13522 gives nhits with a mean of 339.9, rms 13.43
/rat/db/set ELLIE intensity 3000
/rat/db/set ELLIE pulse_mode "poisson"

# Set the wavelength, timing and angular distributions
/rat/db/set ELLIE wavelength_dist "LED434simple"
/rat/db/set ELLIE time_dist "AMELLIE3p0ngauss"
/rat/db/set ELLIE angle_dist "FA3p5deggauss"

/run/initialize

# BEGIN EVENT LOOP
/rat/proc frontend
/rat/proc trigger
/rat/proc eventbuilder
/rat/proc calibratePMT
/rat/proc count

# BEGIN EVENT LOOP

# Output file
/rat/proclast outroot
/rat/procset file "ratoutput AMELIE MCEV Snoplus LED434simple abslengthscale/intensity3000_1_00.root"

# Select LED generator
/generator/add ellie
/generator/rate/set 1

# No of simulated events
/rat/run/start 10000

exit

---

Code A.2: psup_proj.cc  (SNO+ Collaboration)

```cpp
// Vectors For PSUP Projection

#include <TVector3.h>
#include <TVector2.h>
#include <algorithm>
using namespace std;

double fa = 1.0 / 5.5;
double fb = fa * sqrt(3.0) / 2.0;

TVector2 *fA12a = new TVector2( fa / 2.0, 0.0);
TVector2 *fA12b = new TVector2( 3.0 * fa / 2.0, 0.0);
TVector2 *fA12c = new TVector2( 5.0 * fa / 2.0, 0.0);
TVector2 *fA12d = new TVector2( 7.0 * fa / 2.0, 0.0);
TVector2 *fA12e = new TVector2( 9.0 * fa / 2.0, 0.0);
TVector2 *fA2a = new TVector2( 0.0, fb);
TVector2 *fA2b = new TVector2( 5.0 * fa, fb);
TVector2 *fA17a = new TVector2( fa / 2.0, 2.0 * fb);
TVector2 *fA17b = new TVector2( 11.0 * fa / 2.0, 2.0 * fb);
TVector2 *fA51a = new TVector2( fa, 3.0 * fb);
TVector2 *fA51b = new TVector2( 2.0 * fa, 3.0 * fb);
TVector2 *fA51c = new TVector2( 3.0 * fa, 3.0 * fb);
TVector2 *fA51d = new TVector2( 4.0 * fa, 3.0 * fb);
TVector2 *fA51e = new TVector2( 5.0 * fa, 3.0 * fb);
TVector2 *fA37 = new TVector2( 9.0 * fa / 2.0, 2.0 * fb);
```

TVector2 *fA33 = new TVector2( 3.0 * fa / 2.0, 2.0 * fb );
TVector2 *fA58 = new TVector2( 5.0 * fa / 2.0, 2.0 * fb );
TVector2 *fA54 = new TVector2( 7.0 * fa / 2.0, 2.0 * fb );

TVector2 TransformCoord( const TVector3& V1, const TVector3& V2, const TVector3& V3, const TVector2& A1, const TVector2& A2, const TVector2& A3, const TVector3& P )
{
TVector3 xV = V2 - V1;
TVector3 yV = ( ( V3 - V1 ) + ( V3 - V2 ) ) * 0.5;
TVector3 zV = xV.Cross( yV ).Unit();

double planeD = V1.Dot( zV );
double t = planeD / P.Dot( zV );
TVector3 localP = t * P - V1;
TVector2 xA = A2 - A1;
TVector2 yA = ( ( A3 - A1 ) + ( A3 - A2 ) ) * 0.5;
double convUnits = xA.Mod() / xV.Mag();

TVector2 result;
result = localP.Dot( xV.Unit() ) * xA.Unit() * convUnits;
result += localP.Dot( yV.Unit() ) * yA.Unit() * convUnits + A1;
return result;
}

TVector2 Icosahedron( TVector3 pmtPos )
{
TVector3 pointOnSphere( pmtPos.X(), pmtPos.Y(), pmtPos.Z() );
pointOnSphere = pointOnSphere.Unit();
pointOnSphere.RotateX( -45.0 );
const double t = ( 1.0 + sqrt( 5.0 ) ) / 2.0;
const TVector3 V2 = TVector3( t * t, 0.0, t * t * t ).Unit();
const TVector3 V3 = TVector3( -t * t, 0.0, t * t * t ).Unit();
const TVector3 V12 = TVector3( 0.0, t * t * t, t * t ).Unit();
const TVector3 V17 = TVector3( 0.0, -t * t * t, t * t ).Unit();
const TVector3 V27 = TVector3( t * t * t, 0.0, t * t * t ).Unit();
const TVector3 V31 = TVector3( -t * t * t, t * t, 0.0 ).Unit();
const TVector3 V33 = TVector3( -t * t * t, -t * t, 0.0 ).Unit();
const TVector3 V37 = TVector3( t * t * t, -t * t, 0.0 ).Unit();
const TVector3 V46 = TVector3( 0.0, t * t * t, -t * t ).Unit();
const TVector3 V51 = TVector3( 0.0, -t * t * t, -t * t ).Unit();
const TVector3 V54 = TVector3( t * t, 0.0, -t * t * t ).Unit();
const TVector3 V58 = TVector3( -t * t, 0.0, -t * t * t ).Unit();

// Faces { { 2, 6, 17}, { 2, 12, 6}, { 2, 17, 37}, { 2, 37, 27}, { 2, 27, 12}, {37, 54, 27},
// {27, 54, 46}, {27, 46, 12}, {12, 46, 31}, {12, 31, 6}, {6, 31, 33}, {6, 33, 17},
// {17, 33, 51}, {17, 51, 37}, {37, 51, 54}, {58, 54, 51}, {58, 46, 54}, {58, 31, 46},
// {58, 33, 31}, {58, 51, 33} }

vector<TVector3> IcosahedralCentres;
IcosahedralCentres.push_back( ( V2 + V6 + V17 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V2 + V12 + V6 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V2 + V17 + V37 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V2 + V37 + V27 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V2 + V27 + V12 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V37 + V54 + V27 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V27 + V46 + V12 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V12 + V46 + V31 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V12 + V31 + V6 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V6 + V31 + V33 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V6 + V33 + V17 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V17 + V33 + V51 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V17 + V51 + V37 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V37 + V51 + V54 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V58 + V54 + V51 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V58 + V46 + V54 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V58 + V31 + V46 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V58 + V33 + V31 ) * ( 1.0 / 3.0 ) );
IcosahedralCentres.push_back( ( V58 + V51 + V33 ) * ( 1.0 / 3.0 ) );

vector<double> distFromCentre;
unsigned int uLoop;
for( uLoop = 0; uLoop < IcosahedralCentres.size(); uLoop++ ) {
    distFromCentre.push_back( ( IcosahedralCentres[uLoop] − pointOnSphere ).Mag() );
}
const int face = min_element( distFromCentre.begin(), distFromCentre.end() ) − distFromCentre.begin() + 1;
TVector2 resultPosition;
switch(face) {
    case 1:// {2, 6, 17}
        resultPosition = TransformCoord( V2, V6, V17, *fA2a, *fA6, *fA17a, pointOnSphere );
        break;
    case 2:// {2, 12, 6}
        resultPosition = TransformCoord( V2, V12, V6, *fA2a, *fA12a, *fA6, pointOnSphere );
        break;
    case 3:// {2, 17, 37}
        resultPosition = TransformCoord( V2, V17, V37, *fA2b, *fA17b, *fA37, pointOnSphere );
        break;
    case 4:// {2, 37, 27}
        resultPosition = TransformCoord( V2, V37, V27, *fA2b, *fA37, *fA27, pointOnSphere );
        break;
    case 5:// {2, 27, 12}
        resultPosition = TransformCoord( V2, V27, V12, *fA2b, *fA27, *fA12e, pointOnSphere );
        break;
    case 6:// {37, 54, 27}
        resultPosition = TransformCoord( V37, V54, V27, *fA37, *fA54, *fA27, pointOnSphere );
        break;
    case 7:// {27, 54, 46}
        resultPosition = TransformCoord( V27, V54, V46, *fA27, *fA54, *fA46, pointOnSphere );
        break;
    case 8:// {27, 46, 12}
        resultPosition = TransformCoord( V27, V46, V12, *fA27, *fA46, *fA12d, pointOnSphere );
        break;
    case 9:// {12, 46, 31}
        resultPosition = TransformCoord( V12, V46, V31, *fA12c, *fA46, *fA31, pointOnSphere );
        break;
    case 10:// {12, 31, 6}
        resultPosition = TransformCoord( V12, V31, V6, *fA12b, *fA31, *fA6, pointOnSphere );
        break;
    case 11:// {6, 31, 33}
        resultPosition = TransformCoord( V6, V31, V33, *fA6, *fA31, *fA33, pointOnSphere );
        break;
    case 12:// {6, 33, 17}
        resultPosition = TransformCoord( V6, V33, V17, *fA6, *fA33, *fA17a, pointOnSphere );
        break;
    case 13:// {17, 33, 51}
        resultPosition = TransformCoord( V17, V33, V51, *fA17a, *fA33, *fA51a, pointOnSphere );
}
break;
    case 14://{17, 51, 37}
        resultPosition = TransformCoord( V17, V51, V37, *fA17b, *fA51e, *fA37, pointOnSphere );
        break;
    case 15://{37, 51, 54}
        resultPosition = TransformCoord( V37, V51, V54, *fA37, *fA51d, *fA54, pointOnSphere );
        break;
    case 16://{58, 54, 51}
        resultPosition = TransformCoord( V58, V54, V51, *fA58, *fA54, *fA51c, pointOnSphere );
        break;
    case 17://{58, 46, 54}
        resultPosition = TransformCoord( V58, V46, V54, *fA58, *fA46, *fA54, pointOnSphere );
        break;
    case 18://{58, 31, 46}
        resultPosition = TransformCoord( V58, V31, V46, *fA58, *fA31, *fA46, pointOnSphere );
        break;
    case 19://{58, 33, 31}
        resultPosition = TransformCoord( V58, V33, V31, *fA58, *fA33, *fA31, pointOnSphere );
        break;
    case 20://{58, 51, 33}
        resultPosition = TransformCoord( V58, V51, V33, *fA58, *fA51b, *fA33, pointOnSphere );
        break;
    }
    // 1 − x,y pos to project the same as node map
    return TVector2(1.0 − resultPosition.X(), 1.0 − 2.0 * resultPosition.Y() );
}

Code A.3: MCEVcategoriesHistogram.C (excerpt)

RAT::DU::DSReader dsreader(pathname);
RAT::DU::PMTInfo& pmtInfo = RAT::DU::Utility::Get()->GetPMTInfo();
RAT::DU::LightPathCalculator& lpcalc = RAT::DU::Utility::Get()->GetLightPathCalculator();

// Loop through Entries
for (int iEntry = 0; iEntry < dsreader.GetEntryCount(); ++iEntry) {
    RAT::DS::Entry& ds = dsreader.GetEntry(iEntry);
    RAT::DS::MC& mc = ds.GetMC();
    size_t mcTrackCount = mc.GetMCTrackCount();
    size_t mcPMTCount = mc.GetMCPECount();
    size_t mcPCECount = mc.GetMCPECount();

    // Allocate lists to store MC PMT PE info
    UInt_t* mcMCPMTEPMTID_list = new UInt_t[mcPCECount];
    Bool_t* mcMCPMTENoise_list = new Bool_t[mcPCECount];
    UInt_t* mcMCPMTEPhotonTrackID_list = new UInt_t[mcPCECount];

    // Allocate lists to store MC Track info
    UInt_t* mcTrackID_list = new UInt_t[mcTrackCount];
    std::string* mcFirstTrackStepStartVolume_list = new std::string[mcTrackCount];
    ULong64_t* mcTrackSummaryFlag_list = new ULong64_t[mcTrackCount];

    // Position and kinetic energy of initial particle,
    // effectively fibre position.
    const TVector3 mcpPos = mc.GetMCParticle(0).GetPosition();
    const Double_t mcpKE = mc.GetMCParticle(0).GetKineticEnergy();

    // MC Track
for ( size_t iTrack = 0; iTrack < mcTrackCount; ++iTrack ) {
    RAT::DS::MCTrack mcTrack = mc.GetMCTrack(iTrack);

    // Storing Track ID and ULong64_t of Summary Flag
    mcTrackID_list[iTrack] = mcTrack.GetTrackID();
    mcFirstTrackStepStartVolume_list[iTrack] = mcTrack.GetFirstMCTrackStep().GetStartVolume();
    mcTrackSummaryFlag_list[iTrack] = mcTrack.summaryFlag.GetULong64_t(0);
} // end MC Track

// MC PMT
int MCPMTPEiterator = 0; // Used to iterate through all MC PMT PE in all PMTs
for ( size_t iPMT = 0; iPMT < mcPMTCount; ++iPMT ) {
    RAT::DS::MCPMT mcMCPMT = mc.GetMCPMT(iPMT);

    UInt_t mcMCPMTID = mcMCPMT.GetID();
    size_t mcMCPMTPECount = mcMCPMT.GetMCPECount();

    // MC PE
    for ( size_t iPMTPE = 0; iPMTPE < mcMCPMTPECount; ++iPMTPE ) {
        RAT::DS::MCPE mcMCPMTPMPE = mcMCPMT.GetMCPE(iPMTPE);

        Bool_t mcMCPMTPENoise = mcMCPMTPMPE.GetNoise();
        if ( mcMCPMTPENoise ) {
            // If MC PMT PE is noise store the Photon track ID as 0.
            mcMCPMTPEPMTID[iPMTPE] = mcMCPMTID;
            size_t mcMCPMTPENoise list[iPMTPE] = mcMCPMTID;
        }
        else{
            // IF MC PMT PE is not noise store Photon track ID.
            mcMCPMTPEPMTID[iPMTPE] = mcMCPMTID;
            mcMCPMTPENoise list[iPMTPE] = mcMCPMTID;
        }
    }
} // end MC PE

// EV //
for ( int iEv=0; iEv < ds.GetEVCount(); ++iEv ) {
    RAT::DS::EV ev = ds.GetEV(iEv);

    // EV CalPMTs
    RAT::DS::CalPMTs evCalPMTs = ev.GetCalPMTs();
    size_t evCalPMTsCount = evCalPMTs.GetCount();

    // EV PMT Cal
    for ( size_t iPMT = 0; iPMT < evCalPMTsCount; ++iPMT ) {
        RAT::DS::PMTCal evCalPMTsPMT = evCalPMTs.GetPMT(iPMT);

        UInt_t evCalPMTsPMTID = evCalPMTsPMT.GetID();
        if ( evCalPMTsPMTID ) {
            // Get the position of the PMT
            TVector3 evPMTpos = pmtInfo.GetPosition(evCalPMTsPMTID);
            // Calculate the PMTs PSUP position
TVector2 icosProj = IcosProject(evPMTpos);

// Residual time Calculation:
lpcalc.CalcByPosition(mcpPos, evPMTpos, mcpKE);
Double_t d_InnerAV = lpcalc.GetDistInInnerAV();
Double_t d_AV = lpcalc.GetDistInAV();
Double_t d_Water = lpcalc.GetDistInWater();

Double_t n_InnerAV = lpcalc.GetInnerAVRI(mcpKE);
Double_t n_AV = lpcalc.GetAVRI(mcpKE);
Double_t n_Water = lpcalc.GetWaterRI(mcpKE);

Double_t theta = mcpPos.Angle(evPMTpos);
Double_t costheta = TMath::Cos(theta);

Double_t rawtime = evCalPMTsPMT.GetTime();
Double_t calctime = (1.0/c) * (d_InnerAV*n_InnerAV + d_AV*n_AV + d_Water*n_Water);

Double_t restime = rawtime - calctime;
// end restime calc

int pe_nr = 0; // PE iterator

// MC PEs
for ( int imcPE = 0; imcPE < mcPECount; ++imcPE ) {
    // Check if the current MC PE PMT ID is the same as the current EV PMT ID
    if ( mcMCPMTPEPMTID_list[imcPE] == evCalPMTsPMTID ) {
        pe_nr += 1; // Signal PE found
    } // end test MC PE PMT ID == EV PMT ID
} // end MC PEs

int isnoise = 1; // Noise flag

// Check number of PEs for current PMTCal
if ( pe_nr ) {
    // MC PEs
    for ( int imcPE = 0; imcPE < mcPECount; ++imcPE ) {
        // Check if MC PE is noise
        if ( mcMCPMTPENoise_list[imcPE] == 0 ){
            // Check if the current MC PE PMT ID is the same as the current EV PMT ID
            if ( mcMCPMTPEPMTID_list[imcPE] == evCalPMTsPMTID ) {
                isnoise = 0;
            }
        }
    }
    // MC Track
    for ( int imcTrack = 0; imcTrack < mcTrackCount; imcTrack++ ){
        // Check if current Track ID is same as current MC PE Photon Track ID
        if ( mcMCPMTPEPhotonTrackID_list[imcPE] == mcTrackID_list[imcTrack] ) {
            *** Fill HitOther category histograms ***

            // Check if current Track ID has summary flag for only HitPMT
            if ( mcTrackSummaryFlag_list[imcTrack] == HitPMT ) {
                if ( mcFirstTrackStepStartVolume_list[imcTrack].compare("cavity") == 0 ) {
                    *** Fill HitPMT category histograms ***
                }
            }
        }
    }
}
else {
    *** Fill HitOpReemission category histograms ***
}
// Check if current Track ID has summary flag for only HitConc
if ( mcTrackSummaryFlag_list[imcTrack] == HitConc ) {
    if ( mcFirstTrackStepStartVolume_list[imcTrack].compare("cavity") == 0 ) {
        *** Fill HitConc category histograms ***
    }
    else {
        *** Fill HitOpReemission category histograms ***
    }
}
// Check if current Track ID has summary flag for HitPMT or HitConc
if ( (mcTrackSummaryFlag_list[imcTrack] == HitPMT) || (mcTrackSummaryFlag_list[imcTrack] == HitConc) ) {
    if ( mcFirstTrackStepStartVolume_list[imcTrack].compare("cavity") == 0 ) {
        *** Fill Hit category histograms ***
    }
}
// Check if current Track ID has summary flag for OpReemission
if ( ( mcTrackSummaryFlag_list[imcTrack] & OpReemission ) == OpReemission ) {
    *** Fill HitOpReemission category histograms ***
}
// Check if current Track ID has summary flag for OpRayleigh
if ( ( mcTrackSummaryFlag_list[imcTrack] & OpRayleigh ) == OpRayleigh ) {
    *** Fill HitOpRayleigh category histograms ***
}
// Check if current Track ID has summary flag for OpReemission and OpRayleigh
if ( (( mcTrackSummaryFlag_list[imcTrack] & OpReemission ) == OpReemission ) && ( mcTrackSummaryFlag_list[imcTrack] & OpRayleigh ) == OpRayleigh ) {
    *** Fill HitOpReemRay category histograms ***
}
// end test Track ID MC == PE Photon Track ID
}
// end MC Track
}
// end test if noise
}
// end EV PMTCal
}
// end Entries

---

Code A.4: AMELIE_MCEV_Snoplus_LED434simple_array_abslengthscale.job

```
# Options for the batch system
# These options are not executed by the script, but are instead read by the
# batch system before submitting the job. Each option is preceeded by '#$' to
# signify that it is for grid engine.
#
# All of these options are the same as flags you can pass to qsub on the
# command line and can be **overridden** on the command line. see man qsub for
# all the details
```
#!/bin/bash
#
# The shell used to interpret this script
#
#$ -S /bin/bash
#
# Execute this job from the current working directory.
#$ -cwd
#
#$ -q serial.q
#$ -t 1-9
#
# Job output to stderr will be merged into standard out. Remove this line if
# you want to have separate stderr and stdout log files
#$ -j y
#$ -o output/
#
# Send email when the job exits, is aborted or suspended
#$ -m eas
#$ -M

# Job Script
# Here we are writing in bash (as we set bash as our shell above). In here you
# should set up the environment for your program, copy around any data that
# needs to be copied, and then execute the program
#
# Here we execute usual shell commands like any other shell script. The
# output here will be sent to the job's standard out
echo "Running job script"
#
# Finally we run our executable. Here we are passing the command line argument
# above to the script
#
# Here we have a new environment variable that is only set for array jobs — $SGE_TASK_ID
# This is the value of the task ID for each array job, so if we asked for an
# array job with 10 tasks, then $SGE_TASK_ID will range from 1 to 10
#
# We are using the $SGE_TASK_ID to select particular input files based on their suffix
#
### Input to job:
job_title="AMELLIE_MCEV_Snoplus_LED434simple_abslengthscale"
base_macro="AMELLIE_MCEV_Tracking.mac"
eventnum='10000'
wavelength_dist='"LED434simple"'
geometry='"geo\snoplus.geo"'
#field="/rat\db\set OPTICS[labppo\scintillator] ABSLENGTH_SCALING"

# Remember to set job integers equal to length of array
array=('1000[ 1.0, 1.0, ]', '1000[ 1.11, 1.0, ]', '1000[ 1.25, 1.0, ]', '1500[ 1.0, 1.0, ]', '1500[ 1.11, 1.0, ]', '1500[ 1.25, 1.0, ]', '3000[ 1.0, 1.0, ]', '3000[ 1.11, 1.0, ]', '3000[ 1.25, 1.0, ]')

# Names to be used in filename for specific tasks
array_title=('intensity1000_1.00' 'intensity1000_0.90' 'intensity1000_0.80' 'intensity1500_1.00' 'intensity1500_0.90' 'intensity1500_0.80' 'intensity3000_1.00' 'intensity3000_0.90' 'intensity3000_0.80')

###
output_dir="ratoutput_${job_title}" # Name of output dir based on job title
# Make output dir with log folder inside
mkdir $output
dir
mkdir $output/log

# Filename for macro for specific task, to be removed after run
task_macro="job${JOB_ID}.task${SGE_TASK_ID}.mac"
cp $base_macro $task_macro

# Specifying the number of events/entry
nev_field="/rat\run\start"
neventnum=$(awk '{print $2}' $task_macro)

# Specifying the intensity
intensity_field="/rat/db/set ELLIE intensity"
intensity=$(awk '{print $5}' $task_macro)

# Specifying the geometry file
geo_field="/rat/db/set DETECTOR geo_file"
geo=$(awk '{print $7}' $task_macro)

# Specifying the wavelength distribution
wave_field="/rat/db/set ELLIE wavelength_dist"
wave_dist=$(awk '{print $9}' $task_macro)

# Change field in task macro for specific field for specific task
output_filename_field="/rat\procset file"
output_filename=$(awk '{print $11}' $task_macro)

# Change field in task macro to specify the output filename
outputfile="${output_filename}root" $task_macro

# Filename for logfile to be put in log folder in output dir
logfile=$(awk '{print $11}' $task_macro)

# Run rat with specific task macro and given logfilename in log folder
rat -l "$logfile" $task_macro
rm $task_macro
echo "Finished job script"

---

Code A.5: AMELLIE_MCEV_Tracking.mac  by Lisa Falk (extended by author)

# Brief: Simulate AMELLIE events (for details see below)
#
# This macro simulates AMELLIE events in the configuration
# FAaaa-DD_NN
# FAaaa identifies the fibre
# DD identifies the fibre slot on the SMELLIE/AMELLIE mounting plate
# (can be changed, for cross-checking the installation against data)
# NN is the no of simulated events
#
# Speed up rat initialisation time
/rat/physics_list/OmitMuonicProcesses true
/rat/physics_list/OmitHadronicProcesses true
# Simulate external async (mask 32768) trigger
# This trigger identifies ELLIE events
/rat/db/set DAQ_RUN_LEVEL trigger_mask 32768
/rat/db/set DAQ_RUN_LEVEL trigger_enable 35967

# Define the detector geometry for the simulation
/rat/db/set DETECTOR geo_file "geo/snoplus.geo"

# Edit optics, done by script
### OPTICS FIELD ###

# Store all tracks
/rat/tracking/store full

# Select a fibre
# Options: FA089, FA189, FA073, FA173, FA050, FA150, FB012
# Also: FAx089−00, FAx089−10, FAx089−20; and similarly for the others
/rat/db/set ELLIE fibre_id "FA092"

# Set the number of photons per beam
# For fibre FA089 aiming for mean 343.5, rms 17.08
# Intensity 13522 gives nhits with a mean of 339.9, rms 13.43
/rat/db/set ELLIE intensity 3000
/rat/db/set ELLIE pulse_mode "poisson"

# Set the wavelength, timing and angular distributions
/rat/db/set ELLIE wavelength_dist "LED451simple"
/rat/db/set ELLIE time_dist "AMELLIE3p0nsgauss"
/rat/db/set ELLIE angle_dist "FA3p5deggauss"

/run/initialize

# BEGIN EVENT LOOP
/rat/proc frontend
/rat/proc trigger
/rat/proc eventbuilder
/rat/proc calibratePMT
/rat/proc count
/rat/procset update 1000
# BEGIN EVENT LOOP

# Output file
/rat/proclast outroot
/rat/procset file "AMELLIE_FA092_419_scint_10000_00.root"

# Select LED generator
/generator/add ellie
/generator/rate/set 1

# No of simulated events
/rat/run/start 10000

exit