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A Monte Carlo Study
of the
Sudbury Neutrino Observatory
Small Test Detector Experiment

Alan B. Yeung

January 29, 1990

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"A Monte Carlo Study of the Sudbury Neutrino Observatory
Small Test Detector Experiment"

submitted by

Alan B. Yeung

in partial fulfilment of the requirements for
the degree of Master of Science

Thesis Supervisor

Chair, Department of Physics

CARLETON UNIVERSITY

January 29, 1990

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Abstract

A Monte Carlo study of the Sudbury Neutrino Observatory Small Test Detector Experiment is presented. The Small Test Detector consists of a cylindrical water filled tank with 43 photomultiplier tubes arranged in a cylindrical array facing the center of the tank. Electrons are fired into the center of the tank at energies in the range of 2 - 11 MeV and the response of the PMTs are recorded for single electron events.

The simulated photoelectron yield as a function of incident electron energy; and the angular distributions of PMT response for 3.0, 6.5 and 11.0 MeV electrons show excellent agreement with the experimental results.

events lead one to conclude that the operation of such large underground water Čerenkov detectors is understood in considerable detail.

It had yet to be shown that Monte Carlo simulations of the performance of the two large water Čerenkov detectors could be extrapolated with confidence down to the low energy regime of solar neutrinos events (4 to 14MeV). Since the validity of simulations in this energy regime is crucial in determining the ultimate performance of the SNO detector, the SNO collaboration decided in 1986 to set up a small scale prototype detector (STD) to provide experimental confirmation of our ability to adequately simulate low energy events.

This thesis begins with the background that led up to the SNP which includes topics such as the Davis radiochemical experiment and the Kamiokande II detector. Following that is a discussion of the proposed SNO detector, with emphasis on how SNO proposes to solve the SNP. A brief digression into the subject of neutrino oscillations is given as an alternative theory to the standard solar model. The latter part of this thesis begins with a description of the STD experiment followed by a detailed discussion on the design of the STD simulation. Results of the simulation are presented alongside experimental results and a final discussion follows.

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To J.R., and my little munchkins Jaz & Alex ...

1 Introduction

Traditionally, information about the stars has come from the study of the photons they emit. The problem with this method is that the mean free path of a photon in the interior of a star, where nuclear fusion occurs, is less than a centimeter so that key information like the emission energy is lost. That is why solar neutrino experiments offer a unique way of studying the interior of stars. Neutrinos interact so weakly with matter that they can escape unscathed from the interior of a star. By observing neutrinos from the stars, there is the possibility of directly testing theories concerning the types of nuclear reactions and their rates within these stars.

The first solar neutrino experiment was performed using ^{37}Cl by Ray Davis et al. [1] using the Brookhaven solar neutrino detector at the Homestake gold mine. Using a large tank containing 390,000 liters of liquid tetrachloroethylene, C_2Cl_4 , they counted the number of Ar^{37} atoms created from the reaction $\text{Cl}^{37}(\nu, e^-)\text{Ar}^{37}$. The neutrino flux measured by Davis et al. was a factor three lower than that predicted by the standard solar models [2]. This discrepancy has since become known as the solar neutrino problem (SNP).

The SNP has prompted a variety of solutions ranging from neutrino oscillations [3], to many non-standard solar models [4]. The neutrino oscillation theories postulate that the neutrinos are being created in the predicted quantities, but in transit to Earth change into another type of neutrino.

Since current neutrino experiments measure only the ν_e flux, there is no way of testing this theory. The non-standard solar theories typically postulate a lowering of the Sun's interior temperature, thus lowering the rate of 8B decay neutrinos. In either case there can be no resolution to the SNP with existing neutrino detectors.

To address the SNP, a new detector has been proposed. This detector, known as the Sudbury Neutrino Observatory [5] will give scientist the opportunity to solve the SNP as well as being a first class facility for studying neutrino physics. What makes SNO unique is that it will be able to measure the total neutrino flux and the ν_e flux independent of each other. Measurement of the total neutrino flux tests the standard solar model independent of neutrino oscillations and the ratio of the ν_e flux over the total flux tests the neutrino oscillation hypothesis independent of the standard solar model.

Currently there are two large scale underground water Čerenkov detectors, one operated by the IMB collaboration and the second at Kamioka in Japan. Both were originally designed for the study of nucleon decay experiments, but since 1987 the Kamioka detector has had its operating range extended to low energies to search for 8B solar neutrinos. Monte Carlo simulations of events have helped greatly in predicting the response of these detectors in real experimental situations. The agreement at higher energies between the simulations and observations for various types of calibration

events lead one to conclude that the operation of such large underground water Čerenkov detectors is understood in considerable detail.

It had yet to be shown that Monte Carlo simulations of the performance of the two large water Čerenkov detectors could be extrapolated with confidence down to the low energy regime of solar neutrinos events (4 to 14 MeV). Since the validity of simulations in this energy regime is crucial in determining the ultimate performance of the SNO detector, the SNO collaboration decided in 1986 to set up a small scale prototype detector (STD) to provide experimental confirmation of our ability to adequately simulate low energy events.

This thesis begins with the background that led up to the SNP which includes topics such as the Davis radiochemical experiment and the Kamiokande II detector. Following that is a discussion of the proposed SNO detector, with emphasis on how SNO proposes to solve the SNP. A brief digression into the subject of neutrino oscillations is given as an alternative theory to the standard solar model. The latter part of this thesis begins with a description of the STD experiment followed by a detailed discussion on the design of the STD simulation. Results of the simulation are presented alongside experimental results and a final discussion follows.

2 The Solar Neutrino Problem

To date, only two experiments have reported measurements of the flux of solar neutrinos. Both have reported a flux much lower than that predicted by the standard solar models to date [2]. The first was the *Cl/Ar* radiochemical experiment performed by Ray Davis et al. [1] using the Brookhaven solar neutrino detector operating at the Homestake gold mine since 1968. They reported a ^{37}Ar production rate [1] above background of 0.38 ± 0.05 atoms per day. Comparing this to the 1.6 ± 0.5 atoms per day predicted for this experiment by SSM [2], the value reported by the Davis experiment is a factor three lower. More recently, experimenters at Kamiokande II have reported an upper limit of $3.2 \times 10^6 \text{cm}^{-2}\text{s}^{-1}$ for the ^8B flux. Again, this is factor two lower than that predicted by SSM. The measurement at Kamiokande II is also important because it gives independent experimental support for a lower ^8B ν_e flux than predicted by SSM.

3 The Standard Solar Model

Before going any further it is perhaps instructive to describe what is meant by the “standard solar model”, and briefly, how it is derived and how it calculates the present neutrino flux.

Basically, the SSM is the result of the best physics and input parameters available at the time the model is constructed. Thus the set of numbers that corresponds to the SSM vary with time and hopefully converges on

true SSM.

The most important input data used in the constructing SSMs are nuclear cross sections, the solar luminosity, the solar age, the equation of state, the elemental abundances, and the radiative opacity. The best estimates of these parameters can be found in Bahcall's paper [2].

The general procedure of constructing SSMs is begun by guessing an initial set of input parameters. The models are then marched along in time using difference equations to represent the equations of stellar evolution. The predicted characteristics of the present sun are then calculated and the whole processes is iterated until there is good numerical agreement between the model and the observed sun. i.e. parameters such as solar luminosity and solar radius.

The neutrino fluxes are finally calculated from information given by the SSM. i.e. The elemental abundances in the solar interior, the temperature, the density and our knowledge of reaction cross sections. Table 1 shows the neutrino flux for the various sources for the standard solar model.

What are non-standard models? Non-standard solar models are, by definition, constructed by changing something, such as the physics or the input data, from the current or best guess to something less plausible. Most of the non-standard models that have been published were invented to solve the SNP, one of which is the topic of the next section.

Table 1: Neutrino fluxes for the standard solar model [2].

Source	Flux ($10^{10} cm^{-2} sec^{-1}$)
pp	6.0
pep	1.4×10^{-2}
hep	7.6×10^{-7}
7Be	4.7×10^{-1}
8B	5.8×10^{-4}
${}^{13}N$	6.1×10^{-2}
${}^{15}O$	5.2×10^{-2}
${}^{17}F$	5.2×10^{-4}

4 Neutrino Oscillations

One explanation of the SNP put forward in 1964 by Pontecorvo [3], is the topic of neutrino oscillations. The neutrino oscillation hypothesis suggests that neutrinos created in one state can oscillate into another. The basis for this hypothesis is that neutrinos emitted in weak decay are not mass eigenstates, but are linear combinations of neutrino mass eigenstates. More recently, Mikheyev and Smirnov [6] have taken Wolfenstein's work [7] one step further and have shown that these oscillations may be greatly enhanced by dense matter, such as that found in the core of a star.

To illustrate this point, consider the case of the two neutrino types ν_e and ν_μ . Oscillations occur if the eigenvectors of the mass matrix are mixtures:

$$\nu_e = \nu_1 \cos \theta + \nu_2 \sin \theta \quad (1)$$

$$\nu_\mu = -\nu_1 \sin \theta + \nu_2 \cos \theta \quad (2)$$

where ν_1 and ν_2 are the neutrino mass eigenstates with masses m_1 and m_2 .

If a ν_e is produced, then the probability of it being a ν_μ is:

$$P(\nu_e \rightarrow \nu_\mu) = 1 - \sin^2 2\theta \sin^2 \left(\frac{1.27 \Delta m^2 L}{E} \right) \quad (3)$$

where Δm^2 equals $m_1^2 - m_2^2$ measured in eV^2 , E is the energy in MeV and L is the distance in meters.

Two types of experiments have been carried out to search for vacuum oscillations. The flux of $\bar{\nu}_e$ at various distances from a reactor have been measured to determine if the oscillations of the $\bar{\nu}_e \rightarrow \nu_\mu$ [8] occur in the quantities predicted by the above. No evidence of neutrino oscillations was found, but with distances of order 50m, the experimenters were able to rule out values of $\Delta m^2 > 10^{-2} eV^2$ for large mixing angles. Experiments have also been carried to measure the vacuum oscillations of $\nu_\mu \rightarrow \nu_e$ [9]. Again no evidence of oscillations was found.

5 The Cl-Ar Radiochemical Detector

The first solar neutrino experiment was performed in 1968 using ^{37}Cl by Ray Davis et al. [1] using the Brookhaven solar neutrino detector located at the Homestake gold mine. It was this landmark experiment that measured the neutrino flux to be a factor three lower than that predicted by the standard solar models [2].

The detector consists of a cylindrical tank containing 390,000 liters of liquid tetrachloroethylene, C_2Cl_4 . The detector is located 4850 feet (4400 mWe) underground. The neutrino flux is measured by counting the number of ^{37}Ar atoms produced in the neutrino capture reaction:

Neutrino detection depends upon removing the ^{37}Ar from a large volume of liquid contained in a sealed tank, and observing the decay of ^{37}Ar (35-day half-life) in a small proportional counter ($0.5cm^3$). The fraction of a cm^3 of ^{37}Ar is removed by purging with helium gas.

The current upper limit for the 8B neutrino flux observed by this experiment is

$$\phi({}^8B) \leq 2 \times 10^6 cm^{-2}s^{-1}, \quad (5)$$

which is about three times lower than current best estimate value of $5.8 \times 10^6 cm^{-2}s^{-1}$ obtained from the standard model [2].

Measurements with the Cl/Ar detector have continued over the past twenty years. More recently, experimenters are collecting data to build up statistics on the possible time dependence of counting rates. Bahcall [10] has suggested that the unusually high counting rates measured by the Cl/Ar detector are caused by solar flares. Another topic under investigation is evidence of a day-night effect caused by the possible regeneration of

electron neutrinos as neutrinos of different types pass through the Earth [11].

6 The Kamiokande II Detector

The Kamiokande II detector [12] is a 3000 ton water Čerenkov detector originally used in proton-decay experiments. In the last few years it has been upgraded to detect neutrinos. One of these experiments was the search for 8B solar neutrinos from the sun. It was this experiment that gave independent experimental support for a lower ${}^8B\nu_e$ flux than predicted by SSM. This experiment was designed to detect neutrinos from the sun by capturing the Čerenkov light emitted by the scattered electrons in the neutrino electron interaction:

$$\nu_e + e^- \rightarrow \nu_e + e^- \quad (6)$$

The Kamiokande II water Čerenkov detector is located at the Kamioka mine in Gifu prefecture in the region of the Japanese Alps. The detector is located 3000 feet underground (2400mWe). The Kamiokande II detector consists of 948 20 inch diameter PMTs placed uniformly around the inner surface facing inward. The total photocathode surface area of all the PMTs is approximately 20% of the total surface area of the 2140-ton fiducial volume. Each PMT is shielded against magnetic fields, and the tank is surrounded by coils in which currents are passed to cancel out the measured

Earth's magnetic field. An elaborate water purification system ensures that the attenuation length of the tank water for Čerenkov radiation (300 – 500nm) exceeds 50m at any time. In addition, since September 1986, ion exchange columns have maintained the uranium and radium content in the tank water at less than $10^{-3}pCi/liter$, corresponding to less than $10^{-2}Hz$ trigger rate. A 4π solid-angle Čerenkov counter with 123 0.5m diameter PMTs facing outwards is used as an anti-counter. The anticounter layer surrounds the inner detector and the mean thickness of the anti-counter water is 1.5 meters. The anti-counter layer is useful for shielding gammas and neutrinos entering the detector as well as for vetoing cosmic ray muons.

The system records signals larger than 0.35 photoelectrons. The trigger is formed by at least 20 PMT's within 100nsec, which corresponds to 7.5MeV for electrons.

Data collection lasted 208 days. The average trigger rate was 1.2Hz with 0.37Hz due to cosmic ray muons. This should be compared with the expected rate of 0.2 events/day/680 tons ($> 10MeV$) [10]. The large background put extra demands on the experimenters in the data analysis. These demands required the experimenters to select events using the following criteria:

1. Require the total number of photoelectrons be less than 100, which would correspond to an event of less than 30 MeV.
2. Require the total number of anti-counter photoelectrons be less than

30.

3. Require the time interval between events to exceed $100\mu s$ to remove muon decay electrons.
4. Reconstruct the vertex and apply fiducial volume cut to remove events originated by gammas or neutrons entering the detector.
5. Apply directional correlation to the sun to remove events not originating from the sun.

The experimenters (Hirata et al.) at Kamiokande II have given an upper limit at the 90% confidence level for the flux of 8B neutrino of

$$\phi({}^8B) \leq 3.2 \times 10^6 cm^{-2}s^{-1}. \quad (7)$$

This upper limit is about half the value predicted by the SSM [10] of $5.8 \times 10^6 cm^{-2}s^{-1}$.

The biggest problem with the Kamiokande detector is the large background. From the vertex distribution of events it is evident that a large number of events come from the edges of the detector, limiting the fiducial volume of the detector to the central 680 tonnes. Background due mainly to radioactivity inside the water limits the detection threshold to $10MeV$.

7 The SNO Detector

The proposed Sudbury Neutrino Detector will be a 1000 ton D_2O Čerenkov detector, located 6800 feet below ground in the Creighton Mine which is owned by INCO Limited, in the town of Walden near Sudbury. The 1000 tons of D_2O will be contained within an acrylic vessel, constructed from 5cm thick panels surrounded by 4m of high purity H_2O , and 0.9m of low-activity concrete called sulfurcrete. The sulfurcrete will have radioactivity levels 200 times lower than that of ordinary concrete. Mounted uniformly around the vessel, at a distance of 2.5m, are 1995 Hamamatsu R1449 50cm diameter photomultiplier tubes (PMTs), providing 40% photocathode coverage. The PMT array will be sensitive to the Čerenkov radiation produced by relativistic electrons and muons in the central region of the tank.

The SNO detector will exploit five reactions to measure the ν_e flux, energy spectrum and direction, the $\bar{\nu}_e$ flux and energy spectrum, and the total neutrino flux independently of neutrino type.

The ν_e flux, spectrum, and direction will be measured via the charged-current reaction

$$\nu_e + d \rightarrow p + p + e^- \quad (8)$$

corresponding to the ‘inverse beta decay of the deuteron’. In the charged current reaction, the electron-neutrino will be detected by its interaction with the deuteron to form two protons and a electron which carries off

most of the energy. By measuring the energy of the electron, the neutrino spectrum can be deduced. From this, spectral distortions due to neutrino oscillations in the sun can be measured.

The second reaction producing a detectable signal is the neutrino electron scattering

$$\nu_e + e \rightarrow \nu_e + e \quad (9)$$

This reaction involves elastic scattering of neutrinos off electrons, and provides directional information on the neutrinos and will confirm that the observed neutrinos are from the sun.

The total neutrino flux, independent of neutrino type, can be measured by the neutral current reaction

$$\nu_x + d \rightarrow \nu_x + p + n \quad (10)$$

In this reaction, all neutrino types scatter inelastically to break up the deuteron into a proton and a neutron. The main characteristics of this reaction are γ -rays emitted by the subsequent capture of the free neutron. From this, the total neutrino flux can be measured. Therefore, the relative rates of the first reaction and this reaction establishes if conversion of one type of neutrino into another is responsible for the Solar Neutrino Problem.

The fourth and fifth reactions illustrate how SNO will detect the $\bar{\nu}_e$. Although the sun is not expected to be a source of these neutrinos, other

sources like supernovae can be investigated by the reaction

$$\bar{\nu}_e + d \rightarrow n + n + e^+ \quad (11)$$

The signature for this reaction will be the positron signal followed by two delayed neutron capture γ -rays coming from within the D_2O volume.

The fifth reaction will also detect $\bar{\nu}_e$ but this in the surrounding H_2O via the reaction

$$\bar{\nu}_e + p \rightarrow n + e^+ \quad (12)$$

The signature will be the Čerenkov light from the positron, of energy $E_\nu - 1.8MeV$, in the light water. The neutron will be captured in hydrogen giving a $2.2MeV$ γ -ray which will be below the normal detection threshold. The positron direction is almost isotropic with respect to neutrino direction.

As a result of SNO's sensitivity (over forty times that of existing detectors), it will be able to measure the 8B flux at much lower thresholds than attainable by current detectors. Measurements at these lower thresholds can establish if the results of the Davis experiment is compatible with no 8B solar neutrino flux, since the ^{37}Ar could be produced by the background cosmic neutrino flux.

Another advantage of SNO is that it can take data in real time unlike the Cl/Ar radiochemical experiment. By taking data in real time with high statistical accuracy, SNO could provide answers to questions like the

correlation between neutrino flux and solar flares, and the question of the day-night effect caused by the possible regeneration of electron neutrinos as neutrinos of different types pass through the Earth [11].

SNO is also well suited to search for neutrino oscillations. The charged-current reaction (8) will give high statistics data on the ν_e spectrum. The results of which will give immediate support to the matter oscillation hypothesis as it expects gross distortions in the ν_e spectrum. The neutral-current reaction (10) gives the total neutrino flux independent of any oscillation scenario, and combined with the measurement of the ν_e flux from reaction (8), determines in a completely model independent way whether neutrino oscillations are responsible for the SNP.

8 Description of the STD Experiment

This small test detector [13] consists of a water-filled, blackened interior tank 120cm in diameter and a 120 cm in height, with a removeable lid. In total, 43 12.7cm diameter hemispherical PMTs (EMI 9870) were placed inside the cylindrical tank. The original design called for 44 PMTs, but the experimenters found it necessary to remove one of the PMTs to make room for the beam pipe.

Figure 1 shows a schematic of the STD. Twenty-nine of the 43 PMTs form a cylinder around the central axis at a distance of 34 cm. On the top of the tank are seven PMTs arranged in a plane 30.5cm above the center of the tank. The remaining seven PMTs are arranged in a similar way 30.5cm below the center of the tank. The PMTs point inward towards a central cylindrical volume 55cm in diameter and 61cm high. The tubes are regularly spaced and provide approximately 30% coverage. Halfway up the tank a 7.5cm diameter horizontal tube extends into the center of the tank and terminates in a 0.075mm thick brass window. The linac beam line extends into the reentrant tube so that the electron beam is conveyed into the center of the tank with the minimum of scattering and defocussing. The tank is supported at the appropriate height by a framework mounted on a trolley and guide rail arrangement so that it can be backed away from the beam line as required. A waterproof assembly, consisting of a thin plastic scintillator 10mm in diameter and 1.6mm thick optically coupled to a small

Figure 1: Schematic of the Small Test Detector. The beam line from the LINAC extends into the center of the tank.

13mm PMT via a right angle light pipe, is mounted on to the reentrant tube to provide a gating signal from the incident linac electrons.

Figure 2 shows a schematic of the electronic circuitry. The output signal line from each of the 43 PMTs is terminated with 50ohms and fed into a variable gain amplifier ($\times 3 \rightarrow \times 10$). The amplified signals are then fed via 64ns delay lines into LeCroy type multichannel analog-to-digital (ADC's) converters which are plugged into a CAMAC crate controlled by a PDP11/34 minicomputer. The amplified and shaped signal from the plastic scintillator triggers a fast discriminator which generates a 100ns pulse used to gate the ADC's; the 100ns gate pulse triggers a 1 μ s wide pulse which is routed to the 'strobe' input of the CAMAC crate controller. The scintillator analog signal is also fed via 32ns delay into one of the ADC channels.

The computer peripherals include a display terminal, an 800BPI tape drive, dual floppy disc units and a printer. The data is written on tape in 50 event blocks; for each event a sequence number, the time to 1/60th of a second, and the digital output of the 48 ADC channels are recorded. The PDP11/34 runs a multitasking operating system which allows simultaneous running of several programs to process and display the event data on line as they are being recorded.

The experiment was run from the spring to the summer of 1987. The typical procedure was to fill the tank with 1300 liters of distilled water before each run. Samples were drawn off at frequent intervals to monitor

Figure 2: Electronics block diagram for linac runs.

the optical quality of the water which tended to deteriorate with time due to the corrosion of the tank and PMT support framework. The water was removed at the end of every working day and stored in polythene vats until the next run.

Runs were made at six beam energies corresponding to the following electron energies on entering the water: 2.3, 2.8, 3.8, 5.8, 7.6 and 10.3 *MeV*. Four runs were made at each energy: two with the PMT high voltage at the nominal setting, and two with the PMT high voltage at nominal+100V; at each high voltage setting one run was made with the 100ns wide gate pulse ‘normal’, i.e. prompt, and one with the gate pulse delayed by 300ns to measure background. Ten thousand events were recorded in each run.

9 Monte Carlo Design of the STD

The following sections discuss the Monte Carlo design of the main components that make up the SNO-STD simulation.

9.1 Program Flow

The simulation breaks down the electron’s trajectory into small steps or cells, and at each step the following is done:

1. A check is made to see if the electron undergoes Bremsstrahlung. If so, the momentum and energy of the deflected electron and photon are calculated and the simulation continues as normal. Processing of

the photon is deferred until the current electron's energy falls below the Čerenkov cutoff energy of 0.773MeV .

2. The multiple scattering angles are calculated and the electron's momentum is updated.
3. The energy loss due to ionization is calculated and the electron's energy is updated.
4. The number of Čerenkov photons emitted is calculated. The trajectory of each Čerenkov photon is determined, and the response of each PMT hit is recorded.

At the beginning of each step, a check is made to see if the electron's energy has fallen below the Čerenkov cutoff energy. i.e. the energy below which the electron does not emit any Čerenkov radiation. When the electron energy falls below this cutoff, the event is over, and any deferred photons created previously by Bremsstrahlung are then processed.

Photons are simulated in a similar way to the electrons. At each step or cell, the two tests are performed until the photon is either annihilated or escapes the chamber.

1. A test is made to see if Compton scattering has occurred.
2. A test is made to see if pair production has occurred.

In the case where both test positive, a weighted dice is rolled to determine which process takes place. The weighting is a function of the probabilities of that particular process occurring.

When there are no more deferred photons, the whole process is repeated for the next event until there are no more events to simulate, at which point various statistics are compiled and saved onto disk in the form of an ASCII text file.

9.2 The Electron Beam

This section deals with the design aspects that went in the simulation of the LINAC. The SNO-STD experiment used the NRC's electron linear accelerator (LINAC) to produce the required mono-energetic beams.

Modelling the beam is not as straight forward as firing mono-energetic electrons into the tank because, in reality, the electrons were only nearly monoenergetic with a 0.25MeV standard deviation. To reflect this, the simulation folds in a Gaussian distribution with a mean equal to the beam energy and a standard deviation of 0.25MeV .

It should be borne in mind that although the initial beam energy is allowed to fluctuate, it's initial position and direction are not. That is, the starting position and direction of every electron that is simulated is still identical. In essence, the simulation models the statistical fluctuations of the beam energy but not the momentum.

The last step in modelling the LINAC was to simulate the electron

scatter through the scintillator located on the end of the beampipe. This 1.6 mm thick, 10 mm diameter plastic scintillator provided a gating signal in the experiment but serves no purpose in the simulation except as a scatterer. This is simulated by letting the electrons scatter through a water equivalent thickness of the scintillator.

No attempt was made to simulate the Čerenkov light that is emitted as the electrons cross through the scintillator. This is because rough calculations showed that if they are considered the Čerenkov light that will be released would make up only 1.3% of the total Čerenkov photons emitted for a 10 MeV electron, and can be ignored with little impact on the accuracy of the model.

9.3 The Electromagnetic Interactions

The following subsections deal with the modelling of the electromagnetic interactions that occur as a result of the electrons entering the water. The topics that follow include: Multiple scattering, Bremsstrahlung, Ionization energy loss, Čerenkov radiation, Compton scattering and pair production by photons. The latter two are the result of the Bremsstrahlung electron ejecting an energetic photon that collides with the H_2O atom.

9.3.1 Multiple Scattering

When the electron traverses a given thickness of a medium it undergoes many small-angle elastic scatters. The bulk of this deflection is due to

elastic Coulomb scattering with the nuclei of the medium, hence the name multiple Coulomb scattering.

The true distribution of the total deflections is roughly Gaussian for only small angle scatters, with a greater probability for large-angle scatters. However, for non-critical applications, the angular distribution is best approximated with the following formula for the width:

$$\theta_0 = \frac{14.1 \text{ MeV}/c}{p\beta} Z_{inc} \sqrt{L/L_R} \left[1 + \frac{1}{9} \log_{10}(L/L_R) \right] (\text{radians}), \quad (13)$$

where p , β , and Z_{inc} are the momentum (in MeV/c), velocity, and the charge number of the incident particle, and L/L_R is the thickness in radiation lengths, of the scattering medium (for water, $L_R = 36.1 \text{ cm}$). According to the Particle Properties Data Booklet [14] page 77, equation(13) is accurate to about 5% for $10^{-3} < L/L_R < 10$. In terms of this simulation, this equation is accurate for cell sizes down to 0.05 cm . The non-projected space and projected plane angle are then related to equation (13) through the following:

$$\theta_0 = \theta_{plane, rms} = \frac{1}{\sqrt{2}} \theta_{space}^{rms} \quad (14)$$

To arrive at a Gaussian distributed random space angle with mean zero and width θ_{space}^{rms} the following formula is used:

$$\theta = \Phi \times \theta_{space}^{rms}, \quad (15)$$

where Φ is a function that returns a normally distributed random number (Mean = 0, $\sigma = 1$).

Hence, the average deflection an electron undergoes when it travels a given thickness of water can be determined for a given cell size.

0.3.2 Bremsstrahlung

Bremsstrahlung is the process whereby an incoming charged particle interacts with the atom to produce a single photon of comparable energy. The incoming particle is deflected in the process and suffers a loss of energy equal to the energy of the newly created photon and recoil nucleus. Bremsstrahlung processes are most likely to occur when the electron passes the atom at a distance that is great compared to the nuclear radius and small compared to the atomic radius.

The approach to modeling bremsstrahlung begins by first determining if bremsstrahlung has occurred. Hence, at each step of the simulation bremsstrahlung is said to occur if the following two conditions are satisfied:

1. If a randomly generated number X is less than the ratio of the step size L over the radiation length L_{H_2O} of water.

$$X < \frac{L}{L_{H_2O}} \quad (16)$$

2. If the energy of the electron E is greater than twice its rest mass.

$$E > 2m_e c^2 \quad (17)$$

If both conditions are satisfied, the momentum of the newly created photon and deflected electron is calculated. For simplicity, it is assumed that the recoil nucleus acquires zero momentum. To calculate these parameters the Bethe-Heitler [15] differential cross-section for energy-loss by radiation is used. The process of determining the momentum of the photon and deflected electron begins by randomly choosing values for the momentum of the photon and deflected electron. These parameters are then substituted into the Bethe-Heitler equation so that the value for the cross-section can be calculated. A random number is then generated and compared to the value for the cross-section. The momentums for the emitted photon and scattered electron are accepted when the random number is less than the cross-section, otherwise a new set of momentums are generated and the process repeated.

When an acceptable value for the momentums are found, the photon's momentum and coordinates are saved. The simulation of the scattered electron continues until it's energy falls below the Čerenkov cutoff. When this occurs, all photons that were created for that event are then processed.

9.3.3 Ionization Energy Loss

In dealing with the ionization loss of the electron, work originally began with the Bethe-Bloch equation:

$$\frac{dE}{dx} = \frac{DZ_{med}\rho_{med}}{A_{med}} \left(\frac{Z_{inc}}{\beta} \right)^2 \left[\ln \left(\frac{2m_e\gamma^2\beta^2c^2}{I} \right) - \beta^2 - \frac{\delta}{2} - \frac{C}{Z_{med}} \right] \{1 + \nu\}, \quad (18)$$

where $D = 4\pi N_A r_e^2 m_e c^2 = 0.3070 \text{ MeV cm}^2/\text{g}$; I, δ, C and ν are phenomenological functions. The δ term represents the density effect contribution to energy-loss. Density effects are not significant until the electron reaches relativistic energies ($> 1.5 \text{ MeV}$). Dealing with energies in the $3\text{--}15 \text{ MeV}$ range, concern for this effect led to the replacement of the Bethe-Bloch equation with an equivalent equation that included an expression for the density effect of water. This equation is the Halpern-Hall equation for ionization energy loss [16]:

$$\frac{dE}{dx} = \frac{A}{\beta^2} \left[B + 2 \ln \frac{p}{\mu c} + \ln T' + 1 - \beta^2 - \delta \right], \quad (19)$$

where for water, $A = 2\pi n e^4 / m c^2 \approx 0.0851$; $B = \ln[mc^2(10^8)/(h\nu')^2] \approx 18.5$ and $T' = \frac{1}{2}[E - mc^2]$ (MeV) the function δ represents the density effect upon the energy loss rate. Plots showing electron ranges for electrons from $5 - 100 \text{ MeV}$ are given in a previous report [17]. As expected, the simulated electron ranges using density correction show better agreement with experimental results than their counterparts without density correction.

The quantity dE/dx in equations(18) and- (19) represent the *mean* energy loss via interactions with the atomic electrons of water in a layer of thickness dx . However, statistical fluctuations can cause the *actual* energy

loss to deviate from this mean value. Thus, electrons of equal energy do not lose the same amount of energy in travelling through an equal amount of water, if the layer of water is thin enough.

For thin layers of water ($< 1\text{cm}$) the actual energy loss follows a distribution that is broad and skewed, being peaked below the mean energy loss, and having a long tail towards large energy losses. This type of distribution has become the Landau distribution ¹, after it's discoverer. As the thickness dx is increased the Landau is smeared out into a Gaussian distribution. Since the injected electrons are followed in steps of 0.1 cm , Landau variations in the energy loss are quite apparent.

The method used in calculating the actual energy loss was taken from Rossi [18] pages 32 to 35.

1. Begin by calculating the most probable energy loss using the equation:

$$\left(\frac{dE}{dx}\right)_{MPEL} = \frac{2Cm_e c^2 z}{\beta^2} \left[\ln \frac{4Cm_e^2 c^4 x}{(1-\beta^2)I^2} - \beta^2 + j \right], \quad (20)$$

The quantities j and b are given in graphical form in Rossi page 33 [18]. Rossi plots j and b as a function of G , given by:

$$G = \frac{2Cm_e c^2 x}{\beta^2 E'_m} \quad (21)$$

where $C = 0.0758\text{cm}^2/\text{g}$, x is the thickness of the absorber and E'_m the maximum transferable energy. For the range of parameters used

¹Actually, it's better described as the Vavilov distribution, a form of the Landau distribution with a truncated tail.

in this simulation G remains small, and the values for j and b given by Rossi remain constant over this range.

2. Calculate the parameter Δ_0 , by means of the equation:

$$\Delta_0 = \frac{2Cm_e c^2 x}{\beta^2} b. \quad (22)$$

Δ_0 has units of energy and is related to the width of the distribution.

3. Much like a Gaussian distribution which is characterized by a mean and standard deviation, the Landau distribution is characterized by a peak (most probable energy loss) and a width related to Δ_0 . Therefore, knowing the mean and the width of the Landau distribution, the problem of calculating the actual energy loss is solved if there is some means of generating Landau distributed random numbers. Typically, this will involve a call to a CERN library function called *RanLan*, which was written by K.S.Kolbig and B.Schorr [19].

$$\left(\frac{dE}{dx} \right)_{AEL} = \Delta_0 * \text{RanLan}(x) + \left(\frac{dE}{dx} \right)_{MPEL} \quad (23)$$

where $\text{RanLan}(x)$ is a function that will generate a Landau distributed random number.

The quantity on the left is the actual energy loss of the electron traversing a material of thickness δx . The right hand term is just equation (20), a modified form of the Bethe-Bloch equation.

One drawback has been introduced in using this formula for the energy loss. In calculating the most probable energy loss in equation- (20), Rossi has ignored the density effect contribution to the energy loss. Fortunately, this is not serious if the electron energy range is confined to those used in the STD experiment (3-15 *MeV*).

9.3.4 Čerenkov Radiation

A charged particle moving with constant velocity can emit radiation if it's velocity is greater than the speed of light c/n in the medium it is travelling through. This remarkable effect is named after it's discoverer, P.A. Čerenkov.

When an energetic charged particle enters a transparent medium, the velocity remains unaltered except for subsequent ionization and radiative losses. However, the electric field associated with the particle's charge and magnetic field associated with the motion of the particle are propagated with a velocity c/n , where n is the refractive index of the medium. The resulting radiation is canceled in all directions if $\beta n < 1$; however, if $\beta n > 1$ there will be one direction θ in which constructive interference takes place. That is, if the velocity of the particle exceeds the velocity of light in the medium, the particle "runs away" from it's own magnetic field. Consequently, all frequencies in which $\beta n > 1$ can be emitted. This Čerenkov radiation is emitted in a conical surface of half angle θ provided that:

$$\sin \phi = \cos \theta = \frac{(c/n)t}{vt} = \frac{1}{\beta n} \quad (24)$$

The Čerenkov angle θ for relativistic electrons in water (H_2O) is 41.4 deg. This is the polar angle the Čerenkov rays make with the electron path.

It was Fermi that first showed that Čerenkov radiation originated from energy transfers from swift particles to distant atoms which is subsequently emitted as coherent radiation.

Frank and Tamm [20] have shown from classical theory that the total energy radiated in a short element of the particle's path dx is:

$$\frac{dE}{dx} = \frac{4\pi z^2 e^2}{c^2} \int \left(1 - \frac{1}{\beta^2 n^2}\right) \nu \delta \nu \quad (25)$$

where ze is the charge on the moving particle and ν is the frequency of the emitted radiation. The same result is obtainable from quantum theory. The integration is to be carried out over all frequencies in which $\beta n > 1$.

The energy lost in Čerenkov radiation is generally small, roughly 10^3 eV per centimeter of glass or lucite, and usually negligible compared to ionization energy losses. Nevertheless this energy is readily detectable because of the relatively large release of ultraviolet radiation.

9.3.5 Compton Scattering

Up to now the discussion has focused on the electromagnetic interactions of the electron with the medium. In this section the focus is shifted towards

the interactions of the energetic photon that is created when the electron undergoes Bremsstrahlung (section 9.3.2). The following sections begin with Compton scattering followed by pair production.

Compton scattering can be described as an elastic collision between a photon and a free electron initially at rest. The *total* probability of a photon of energy E to undergo Compton scattering in a thickness $dx \text{ g cm}^{-2}$ is:

$$\int_{m_e c^2/2}^E \Phi_{com}(E, E') dE' = \frac{C m_e c^2}{E} \left[\ln \frac{2E}{m_e c^2} + \frac{1}{2} \right]. \quad (26)$$

Figure 3 plots the total probability of a photon undergoing Compton scattering as a function of the photon's energy.

Equation(26) is taken from Rossi (page 78 equation (8)) and is valid in the energy range $E \gg m_e c^2$. Figure 3 plots equation (26) the Compton cross section, equation (30) the pair production cross section, their sum and actual experimental data. The results are in good agreement with the experimental data.

Once a Compton collision has occurred, the next task is to determine the scattering angles of the photon and Compton electron. Here, the standard Monte Carlo technique ² is used.

1. Randomly choose the scattered photon angle from 0 to 360 degrees.
2. Calculate the energy E' of the scattered photon using the Compton formula:

²The Von Neumann method. Otherwise known as the acceptance-rejection method.

Figure 3: The total probability for Compton Scattering, pair production as a function of the incident photon's energy. Experimentally determined values are shown along side for comparison.

Figure 3.

$$E' = \frac{Em_e c^2}{m_e c^2 + E(1 - \cos \theta)}, \quad (27)$$

where θ is the scattered photon angle determined in step 1 and E is the incident photon energy.

3. Next, calculate the probability of Compton scattering by substituting the above two values and the energy E of the incident photon into the Klein-Nishina formula:

$$\Phi_{com}(E, E') = \frac{Cm_e c^2}{EE'} \left[1 + \left(\frac{E'}{E} \right)^2 - \frac{E'}{E} \sin^2 \theta \right]. \quad (28)$$

This is the Klein-Nishina differential cross section for Compton scattering. $\Phi_{com}(E, E')$ is the probability of a photon of energy E traversing a thickness dx $g\text{ cm}^{-2}$ undergoing a Compton collision in which the scattered photon has energy E' and angle θ with respect to the incident photon direction.

4. Randomly choose a number between zero and one. If this number is less than the probability calculated in the previous step, accept the values determined in steps 1 and 2 as the scattered photon angle and energy. Otherwise reject them and start again from step 1.
5. Once suitable values for the scattered photon angle and energy are found, use the momentum and energy conservation laws to calculate the angle and energy of the Compton electron.

Do not confuse equations(26) and (28). The former is the *total* probability for a photon of energy E to undergo Compton scattering while the latter is the *differential* probability for a photon of energy E undergoing Compton scattering in which the scattered photon has energy E' and angle θ .

Using equation (28), a plot of the angular distribution of the scattered photon for various incident photon energies is shown in Figure 4. The shape and form of the distributions are very similar to those found in the literature.

9.3.6 Pair Production by Photons

The Compton effect is a phenomena that plays an important role for intermediate and low energy photons ($< 23MeV$). As the photon energy is increased, the Compton effect diminishes but, another phenomenon, called pair production, becomes more prominent.

Pair production is the process whereby an incoming photon interacts with a target particle, creating a positron-electron pair while the target nucleus recoils, and the photon is annihilated. In the case where the nucleus is much more massive than an electron, the sum of the total energies of the positron-electron pair is very nearly the energy E , of the incident photon.

$$E' + E'' + 2m_e c^2 = E, \quad (29)$$

ANGULAR DISTRIBUTION FOR 0.01, 0.05, 0.1, 0.5, 1, 5, 10, 50, 100, 1000 MeV PHOTONS

Figure 4: Angular distribution of the Compton scattered photon for incident photon energies of 0.01, 0.05, 0.1, 0.5, 1, 5, 10 and 100 MeV. equation (28).

where E' and E'' are the kinetic energy of the positron and the electron, respectively.

Let $\Phi_{pair}(E, E')dE'dx$ be the probability of a photon of energy E traversing a thickness $dx \text{ g cm}^{-2}$ to produce a pair, in which the positron has a kinetic energy between E' and $E' + dE'$. That is, Φ_{pair} is the differential probability for pair production.

Integration of $\Phi(E, E')$ from $E' = 0$ to $E' = E - 2m_e c^2$ yields the total probability for a photon with energy E to produce a pair, in thickness $dx \text{ g cm}^{-2}$. In the limit for small energies $m_e c^2 \ll E \ll 137m_e c^2 Z^{-1/3}$, i.e. $0.511 \text{ MeV} \ll E \ll 36 \text{ MeV}$, the integral has the form:

$$\int_0^{E-2m_e^2} \Phi(E, E')dE' = 4\alpha N \frac{Z^2}{A} r_e^2 \left[\frac{7}{9} \ln \frac{2E}{m_e c^2} - \frac{109}{54} \right], \quad (30)$$

where α is the fine structure constant ($\alpha = 1/137$), N is Avagardo's number ($N = 6.022 \times 10^{23}$), and r_e is the classical electron radius ($r_e = 2.817 \times 10^{-13} \text{ cm}$). Equation(30), the total probability for pair production as a function of incident photon energy E , is plotted in Figure 3. Having determined if a photon has undergone pair production with equation(30), the next step is to determine the energies and emission angles of the positron-electron pair.

In determining the energies of the positron-electron pair, the kinetic energy carried off by the positron-electron pair is assumed equal. If this assumption is made, the kinetic energy carried off by the positron E' and

electron E'' is given by:

$$E' = E'' = \frac{E - 2m_e c^2}{2}. \quad (31)$$

In a similar fashion, the emission angles of the positron-electron pair are approximated by the distribution:

$$\theta = \frac{m_e c^2}{E} \quad (32)$$

The simulation then records the position and momentum of the electron and continues the event with this newly created electron. The positron, on the other hand, is ignored. It was assumed that the lifespan of the positron was short in that more often it will (i) recombine with a free electron (annihilation) to form a photon pair of equal energy but opposite in direction, (ii) cause a single photon to be released if it recombined with a tightly bound electron.

Appendix C, proposes a detailed treatment of the pair production phenomena, should the need arise for an alternate treatment of the pair production phenomena.

9.4 PMTs and the Detection of Čerenkov Light

At each iteration of the program, while above the cutoff energy, the electron will generate a number of rays of Čerenkov light. These rays are interpreted as vectors by the program and are passed on to the light detection routines

which determine if a PMT is hit.

To simplify the search process, all PMT's are stored in one data structure called an AVL-tree³. The PMTs are sorted into the AVL-tree by their polar angle. This polar angle is defined as the cosine of the angle between a vector from the center of the tank to the center of the PMT and the x-axis. The x-axis being the beampipe with the origin being the center of the tank.

Once the point of emission and direction of the Čerenkov photon is known, the point of intersection with the chamber is calculated. The next step then is to calculate the polar angle of this point of intersection. Knowing this, the search into the AVL-tree is initiated using the polar angle as the key.

The search begins at the root of the tree and each PMT along the way is checked until either a hit is found or the end of a branch is reached. Since AVL-trees are height balanced, the worst case search will take $O(\log_2 N)$ which is between five and six searches for the case where N is equal to forty-three PMTs. In this experiment with only forty-three detectors the gain in efficiency is small. However, should this design be used in the SNO detector, the improvement would be drastic. For example, should SNO employ 2000 detectors, a PMT hit can be determined with only 11 searches.

The AVL-tree data structure and its supporting routines were easily implemented in the PASCAL language, one of the main reasons why the PASCAL programming language was chosen.

³The Adelson-Velskii and Landis height balanced tree.

The Čerenkov photon is said to be lost to the surroundings if it missed all PMTs. However, if the ray intersects any PMT, two tests are performed to determine the PMT response to the Čerenkov photon. The first test involves the simulation of the individual characteristics of each PMT. In the PMT coordinate file (PMTCOORD.DAT), a experimentally determined parameter ⁴ called "eff" describes the relative detection efficiency of the PMT to a reference PMT. If the photon survives the PMT efficiency cut, the response of the PMT is simulated to determine the number of photoelectrons created by the interaction of the Čerenkov photon with the PMT medium. The PMT's have been simulated so as to have a negative logarithmic response. On average, this will be one photoelectron per Čerenkov photon, but there will be cases where more than one is created, as well as cases where there are none. In the latter case, the interpretation is that the photon is lost because of the poor quantum efficiency of the PMT. The whole process is then repeated for the next photon until all photons are processed for the event.

10 Procedure

Appendix A describes how to run the program, what parameters are needed and their meanings.

The STD experiment was run with incident beam energies in the range

⁴In the STD experiment the response of all PMTs was calibrated to the known response of a 2" PMT

of 2.1- 10.3 *MeV*. The experimental data were corrected for pedestal and accidental coincidence effects by background subtraction. The background measurements were done by recording the PMT response using delayed coincidence (300 ns). The ADC output of the PMTs was converted to 'nominal' photoelectron numbers. 'Nominal' means that the photoelectron numbers have been normalized for efficiency variations among PMTs and are therefore proportional to the number of photons striking the tubes. Details of this can be found in the calibration section of the STD experiment paper [13].

Three energies were selected for comparison. These were at incident electron energies of 2.3, 6.5 and 10.3 *MeV*, covering the middle and two ends of the energy spectrum. From these, the predicted response and observed response of the PMTs were plotted as a function of the polar angle of the PMT for the three energies. In these anisotropy distributions, the simulated responses were, (i) normalized for the solid angle subtended by the PMT at the center of the tank, and (ii) normalized to the experimental response, that is,

$$\sum_{i=1}^{43} N_{pe}^i(MC) = \sum_{i=1}^{43} N_{pe}^i(Expt) \quad (33)$$

where N_{pe}^i is the response in units of photoelectrons of the i th tube.

For the second comparison, the predicted total number of photoelectrons as a function of incident electron energy were plotted alongside the

observed values. Like the STD experiment, all simulated PMT responses were adjusted to the 'nominal' number of photoelectrons.

For the third comparison, the ratio of the central 7 to the forward 21 PMTs as a function of incident electron energy were plotted alongside the observed values to give an indication of the degree of forward peaking.

The simulation was run using 2000 events which consumed just under one hour of VAX CPU time.

11 Results

The STD experiment was run in the energy range of $2 - 11\text{MeV}$. In doing the comparison of the simulation with the STD experiment, results are presented for the anisotropy distributions at incident electron energies of 2.3, 5.8, and 10.3MeV ; as well as the total number of detected photoelectrons as a function of incident electron energy; and the ratio of the central 7 to forward 21 PMTs as a function of incident electron energy.

Firstly, consider the angular distribution of the detected photons. In Figure 5, the mean response of the individual PMTs at 10.3MeV is plotted against the angle subtended at the center of the tank by the beam direction and the center of the PMT face. Each PMT response has been normalized for the solid angle subtended by the PMT at the center of the tank. Similarly, Figures 6 and 7 show the anisotropy distributions for beam energies of 5.8 and 2.3MeV . The simulated and experimental distributions have been normalized such that the sums of the PMT responses for each distribution are equal. At 10.3MeV the simulation shows excellent agreement with experimental data, with both peaking near the Čerenkov angle of 41.2° . The Čerenkov peak is less pronounced at 5.8MeV and is almost smeared out at 2.3MeV . In all three figures, the experimental PMT responses tend to scatter around the simulated responses, especially towards the tail end of the distribution.

Figure 8 shows the total number of detected photoelectrons per event

plotted against the incident electron energy. Again, the simulated data shows excellent agreement with the experimental data.

In Figure 9 the ratio of the central 7 PMTs to the forward 21 PMTs is plotted against the incident electron energy to show the degree of forward peaking of the Čerenkov radiation. In Figure 9 it can be clearly seen that the degree of forward peaking increases steadily with energy.

12 Discussion

Probably the most interesting result of this Monte Carlo simulation is the close agreement between the simulated and experimental results of the numbers of detected photoelectrons, shown in Figure 8. The number of detected photoelectrons is dependent on a parameter called the detectable photons per centimeter of track, which in this simulation is 68. This number, in turn is based on a quantum efficiency rating for the PMTs of 27.2% in the range from 400 to 800 nm and zero outside. The close agreement between the simulation and the experiment in the photoelectron yield leads to the conclusion that the average quantum efficiency of the PMTs used in the experiment to be 27.2% over this range of the spectrum.

This result agrees well with average quantum efficiency for this type of PMT. It is generally understood that this type of PMT exhibits an efficiency curve which peaks in the vicinity of 380nm and falls off steeply on both sides. If the efficiency which is given as a function of the wavelength, is

Figure 5: Mean response of the individual PMTs plotted against the angle subtended at the center of the tank by the beam direction and the center of the PMT face. Responses have been normalized for the solid angle subtended at the center of the tank. Incident electron energy is 10.3 MeV.

Figure 6: Mean response of the individual PMTs plotted against the angle subtended at the center of the tank by the beam direction and the center of the PMT face. Responses have been normalized for the solid angle subtended at the center of the tank. Incident electron energy is 5.8 MeV.

Figure 7: Mean response of the individual PMTs plotted against the angle subtended at the center of the tank by the beam direction and the center of the PMT face. Responses have been normalized for the solid angle subtended at the center of the tank. Incident electron energy is 2.3 MeV.

Figure 8: Mean number of 'nominal' photoelectrons per event for various incident electron energies.

Figure 9: Ratio of the summed response of the central 7 PMTs to that of the forward 21 PMTs for various energies.

integrated over this spectrum, the result for the average efficiency is 28 %.

The results of the anisotropy distributions are shown in Figures 5, 6 and 7, the most important of these being the 10.3MeV case, where at this energy the Čerenkov peaking is most evident. The simulated distribution tends to tail off more rapidly than the experimental results, this may be due to the reflection and scattering of the Čerenkov photons, an effect not considered by the simulation. It is expected that including these effects into the simulation would result in a displacement and broadening of the distribution, but to what extent is unclear.

The results of the simulation as a whole have accurately reproduced the STD experiment. It is felt that the STD simulation has reached a stage of maturity and that further improvements will be met with diminishing returns. The next step now would be to adapt the program to handle a large array of PMTs similar to that of the proposed SNO detector, this should not be as difficult as it sounds as the program was designed to simulate any cylindrical array.

A Running the STD simulation

To run the program the following four files are needed:

1. STD4V05.EXE:

This STD program, the last four characters designate the version number. In this case version 4.05 of the program is used.

2. BATCH.DAT:

The batch file containing the input parameters used by STD4v05 program. The contents of the file are shown in Figure 10. The first parameter is the initial total energy in *MeV* of the electron. The second parameter is the resolution length or cell size of each iteration of the electron. Its units are centimeters. The third parameter is the number of events, that is, the number of electrons to simulate. The fourth parameter applies only to the VAX version, it is the seed for the random number generator. The last parameter is the output file name where the final statistics of the simulation are dumped.

3. PMTCOORD.DAT:

This file contains data specific to the PMTs and is read in once at startup. The coordinates or efficiency of any of PMTs can be changed by modifying this file. Be careful not to overlap any PMTs. The program will not detect this type of error.

Figure 11 shows the actual PMTCOORD.DAT file used in the STD simulation. In this file the first three parameters are identification numbers.

Figure 10: The batch file (BATCH.DAT) containing the input parameters used in the SNO-STD simulation

Input data for STD4v05.PAS, (File BATCH.DAT)

Energy	Resolution	Length	#_of_Events	Seed	Output_File_Name
-----	-----	-----	-----	-----	-----
11.0	0.1		2000	99564	BAT110.OUT

The first of the three is the Id used by this program. The second parameter is the old Id number, which is ignored by the program. The third parameter is the ADC number used by the experimenters. This number allows the PMTs in the simulation to connect with the PMTs used in the experiment. The fourth, fifth and sixth parameters are the cylindrical coordinates of the PMTs in centimeters and degrees (r, ϕ, z). The seventh parameter is the efficiency of the PMT relative to the 2" reference PMT. This is an experimentally determined parameter. The eighth and last parameter is the polar angle of the PMT in degrees. This parameter is ignored by the program since the program calculates the polar angle automatically from the coordinate data of the PMT. It exists only for illustrative purposes.

4. LANDAU.DAT

The data for the function that generates Landau distributed numbers. This file was created from the CERN library function RANLAN. Having studied the paper by Kolbig and Schorr [19], it was quickly realized that there was no simple way of writing such a function. So a lookup table was

used.

A.1 Running in the VAX Environment

With the above four files in the same directory, the program is started by entering:

```
RUN STD4V05
```

It is recommended that a batch file is created containing the above command and submitted onto one of VAX queues for batch processing.

A.2 Running in the IBM-PC Environment

In addition to the four files listed above, the Turbo Pascal 4.0 graphics drivers will be required if graphics are enabled. These drivers will have to be placed in a directory called

```
\TURBO\DRIVERS
```

The type of driver will of course depend on the type of monitor being used, using any other monitor besides a Hercules may have unpredictable results since this simulation has only been run on a Hercules graphics adapter. The simulation is started by entering

```
STD4V05
```

Coordinate Data of				ALL PMT's (File PMTCOORD.DAT).			
#	Old#	PM#	R	PHI	Z	Eff	Theta (Cos-Theta)
1	1	26	33.85	0.0	4.81	0.68	9.9
2	26	12	33.85	0.0	24.05	0.86	41.2
3	11	9	33.85	0.0	-14.43	0.67	27.7
4	6	44	33.85	36.0	-4.81	0.99	37.2
5	16	33	33.85	36.0	14.43	0.75	44.2
6	21	18	33.85	36.0	-24.05	0.91	52.5
7	4	4	33.85	72.0	4.81	0.78	72.3
8	27	5	33.85	72.0	24.05	0.89	76.5
9	12	15	33.85	72.0	-14.43	0.77	74.1
10	8	36	33.85	108.0	-4.81	0.75	107.7
11	18	41	33.85	108.0	14.43	0.61	105.9
12	23	47	33.85	108.0	-24.05	0.80	103.5
13	2	32	33.85	144.0	4.81	0.47	142.8
14	29	7	33.85	144.0	24.05	0.66	127.5
15	14	27	33.85	144.0	-14.43	0.66	135.8
16	20	29	33.85	180.0	14.43	0.0	152.3
17	25	8	33.85	180.0	-24.05	0.59	138.8
18	3	31	33.85	-144.0	4.81	0.46	142.8
19	30	39	33.85	-144.0	24.05	0.0	127.5
20	15	24	33.85	-144.0	-14.43	0.57	135.8
21	9	38	33.85	-108.0	-4.81	0.0	107.7
22	19	30	33.85	-108.0	14.43	0.53	105.9
23	24	46	33.85	-108.0	-24.05	0.68	103.5
24	5	43	33.85	-72.0	4.81	0.55	72.3
25	26	23	33.85	-72.0	24.05	0.74	76.5
26	13	16	33.85	-72.0	-14.43	0.77	74.1
27	7	42	33.85	-36.0	-4.81	0.36	37.2
28	17	34	33.85	-36.0	14.43	0.34	44.2
29	22	25	33.85	-36.0	-24.05	0.65	52.5
30	31	37	0.0	0.0	36.75	0.96	90.0
31	32	35	19.8	17.3	36.75	0.69	58.6
32	34	10	21.3	-41.0	36.75	0.00	64.3
33	36	13	19.4	-96.3	36.75	0.80	93.4
34	37	6	18.2	-163.1	36.75	0.65	119.4
35	35	40	20.5	135.0	36.75	0.83	113.3
36	33	19	19.7	79.7	36.75	0.73	84.4
37	38	2	0.0	0.0	-36.75	0.80	90.0
38	42	45	19.4	-96.3	-36.75	0.66	93.4
39	40	14	21.3	-41.0	-36.75	0.69	64.3
40	39	3	19.8	17.3	-36.75	0.72	58.6
41	41	11	19.7	79.7	-36.75	0.83	84.4
42	43	28	20.5	135.0	-36.75	0.75	113.3
43	44	17	18.2	-163.1	-36.75	0.47	119.4

Figure 11: The PMT data file used in the SNO-STD simulation (PMTCOORD.DAT).

B Interpreting the Output

When the simulation ends, the program compiles the data, computes various statistics and places them in a output file. This section discusses the meaning of the data contained in this output file.

The data in this file can be broken down into ten sections.

Section 1. This section contains miscellaneous items like the date created, consumed CPU time, etc.

Section 2. A summary of the simulation results. Of particular importance here is the total yield of photoelectrons. The acronym S.D. stands for standard deviation.

Section 3. The third section consists of a table titled DETECTOR COUNTS. This is the unmodified PMTs response. The ID# and the polar angle are placed alongside.

Section 4. Similar to Section 3 except the PMTs response have been normalized for the number of events. Coordinate data etc. is included alongside.

Section 5. Same as Section 3 except the PMTs response have been normalized for the number of events and divided by their efficiency. This is the 'nominal' response of the PMTs.

Section 6. Section 6 is titled ANISOTROPY DISTRIBUTION, it shows the histogram of the of anisotropy angle.

Section 7. A histogram of the number of photoelectrons detected in an event.

Section 8. A histogram of the number of counters triggered in an event.

Section 9. A histogram of the energy of photons created in the Bremsstrahlung process.

Section 10. A histogram of the energy of secondary electrons created in the Compton scattering and pair production processes.

Section 11. A histogram of the energy of electrons as they enter the water.

C Pair Production by Photons

In section 9.3.6, the inadequacy of the simulation's treatment of the pair production phenomenon is mentioned. This appendix proposes a more thorough treatment of the problem.

The equations presented here are from Rossi [18] pages 79 to 86 and Bethe and Heitler [15] page 108. The Von Neumann Monte Carlo technique is employed to determine the emission energies and angles of the positron-electron pair.

1. Begin by randomly choosing ν from a uniform distribution between $[0, 1]$. ν represents the fractional energy of the positron and is defined as

$$\nu = \frac{E' + m_e c^2}{E}, \quad (34)$$

where as before, E is the incident photon energy, and E' the energy of the positron.

2. Having chosen ν , and knowing E the incident photon energy, calculate the positron energy E' , given by equation (34).
3. Assume the H_2O nucleus does not recoil appreciably so that the energy transferred to it is negligible. Then, by conservation of energy, calculate the energy E'' of the electron using

$$E'' = E - E' - 2m_e c^2. \quad (35)$$

4. Because pair production is sensitive to the screening effect of the outer electrons, determine the amount of screening from the following:

$$\gamma = 100 \frac{m_e c^2}{E} \frac{1}{\nu(1 - \nu)} Z^{-1/3}, \quad (36)$$

Screening is negligible for the case $\gamma \gg 1$ and becomes more important as $\gamma \rightarrow 0$. The case when $\gamma \approx 0$ is known as complete screening. For a given ν , γ decreases with increasing E .

5. Calculate the differential probability $\Phi(E')$ for a photon of energy E to create a positron of energy E' and an electron of energy E'' by the formula:

$$\Phi(E') = \frac{Z^2 r_e^2}{\alpha E^2} (E'^2 + E''^2 + \frac{2}{3} E' E'') 4 \left(\log \frac{2E' E''}{E m_e c^2} - \frac{1}{2} - c(\gamma) \right) \quad (37)$$

where $c(\gamma)$ is given table 2. According to Bethe and Heitler, the differential probability function given by equation (37), is applicable only for small photon energies $E \ll 137 m_e c^2 Z^{-1/3}$. Since, this roughly translates to $E \ll 36.2 \text{ MeV}$, the condition is satisfied for purposes of this simulation. Bethe and Heitler also provide modified versions of equation (37) in the case of intermediate and high photon energies.

The Von Neumann method requires that the differential probability function given in equation (37) be normalized to unit area. So, equation (37) must be integrated, analytically—if possible—or numerically, and normalized if necessary. i.e.

$$\Phi_{\text{norm}}(E') = \frac{\Phi(E')}{\int_0^{E-2m_e c^2} \Phi(E') dE'} \quad (38)$$

6. Compute a function $\xi(E')$ whose shape completely encloses $\Phi_{\text{norm}}(E')$. Frequently, ξ is a uniform or a sum of uniform distributions which can be generated relatively quickly.

Table 2: Values for the function $c(\gamma)$ in equation (37). From Bethe and Heitler [15]

$c(\gamma)$	0.21	0.16	0.13	0.09	0.065	0.05	0.03	0.02	0.01
γ	2	2.5	3	4	5	6	8	10	15

7. The last step in determining the positron-electron emission energies is to generate u from a uniform distribution between $[0, 1]$, and test if $u \cdot \xi(E') \leq \Phi(E')$. If so, accept E' as the positron energy; otherwise reject E' and start over.

Determining the emissions angles of the positron and the electron by using the formula given in Bethe and Heitler's paper [15]. From this formula, the number of electrons emitted at an angle θ_0 with energy E_0 , is approximately proportional to:

$$\Phi(\theta_0)d\theta_0 = \frac{\theta_0 d\theta_0}{(\Theta^2 + \theta_0^2)}, \quad (39)$$

where $\Theta = m_e c^2 / E_0$. If this function can be inverted such that

$$\theta_0 = \Phi^{-1}(u), \quad (40)$$

where u is a uniformly distributed random number. Then the task of computing the emission angle θ_0 of the electron would be trivial. If the inverse of equation (39) cannot be found then, the acceptance-rejection method (Von Neumann method) would have to be used (see above).

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