ABSTRACT

XU, YANPING. Characterization of Solid Deuterium Ultracold Neutron Source Production and UCN Transport. (Under the direction of Professor A. R. Young).

Ultracold neutrons (UCN) are neutrons with energies below about 330 neV, making it possible to store them in material bottles for relatively extended periods of time (hundreds of seconds) and to utilize them in a variety of experiments. Until recently, the available UCN flux has limited the range of problems which can be addressed with UCN. In 2000, a series of experiments at LANSCE demonstrated that a solid deuterium super-thermal source coupled to a spallation target can potentially provide orders of magnitude improvements in useful UCN density. Since these prototype experiments, a UCN source has been constructed for the UCNA collaboration in Line B at LANSCE, and another solid deuterium source has been designed to operate at the PULSTAR reactor at NC State University based on similar principles. This work will present the initial results and analysis of the LANL UCN source performance and some of the development and design issues for the PULSTAR source. A Monte-Carlo analysis of UCN depolarization measurement has also been included as a UCN transport study.
Characterization of Solid Deuterium Ultracold Neutron Source Production and UCN Transport

By

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Dedication

This dissertation is dedicated to my respected parents and my beloved wife!

献给我的父母和妻子！
Biography

The author of this dissertation was born in Beijing, P. R. China on Oct. 1971. He began his colleague education at the Jilin University in Changchun, and graduated in 1995 with a Bachelor in Physics.

After that, he worked as a research assistant in China Institute of Atomic Energy (CIAE) for five years.

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Chapter 1

Introduction

1.1 An Introduction to Ultracold Neutrons

1.1.1 Neutron Categories

Traditionally, neutrons are categorized by their energy into five or six groups, with most applied physics research utilizing hot, thermal, and cold neutrons (see figure 1.1.1.1). Neutrons with energies higher than hot neutrons are referred as fast neutrons. Neutrons with energies lower than cold neutrons are referred to as very cold and ultra cold neutrons.

Ultracold Neutrons (UCNs) are commonly defined as neutrons with energies below about 335 neV (Fermi potential of $^{58}\text{Ni}$), with velocity below about 8 m/second, or with wavelengths larger than about 500 Å. Because their energies are so low, they are dramatically affected by gravity (the gravitational potential energy near the earth changes by 100 neV per meter) and applied magnetic fields (the $\mu \cdot B$...
interaction gives rise to a potential energy change of 60 neV per Tesla). An extra feature is that they are totally reflected from any angle of some material surfaces. This property permits UCNs to be trapped inside some containers for a time approaching the neutron decay lifetime, ideal for some measurements of the fundamental properties of the neutrons[4,5,8,19,27,28,46,50,61].

![Total reflection under any angle](image)

Figure 1.1.1.2 UCN Reflection

### 1.1.2 Neutron Moderation and Neutron Energy Spectra

After being generated at the neutron source (reactor or spallation neutron source), high energy neutrons are typically coupled to a serial of moderators to produce cold neutron and Ultracold neutrons. In thermal equilibrium with the moderator, neutrons will follow the Maxwell-Boltzmann distribution:

\[
N(E) = \frac{2\pi}{(\pi kT)^{3/2}} \sqrt{E} \exp\left(-\frac{E}{kT}\right),
\]

(1.1)

Where \(N(E)\) is the number of neutrons within the unit volume and unit energy interval, \(E\) is the energy of the incident neutron, \(T\) is the temperature of the moderator. So the moderated neutron flux depends on the temperature of the moderator.
Figure 1.1.2.1 shows un-normalized neutron flux vs. neutron energy at different temperatures. The typical cold neutron source is a specially designed container which holds low temperature moderator to slow down neutrons.

![Figure 1.1.2.1 Neutron Moderation](image)

### 1.2 Superthermal UCN Source

As mentioned in section 1.1, UCN have some advantages for fundamental neutron physics research. For example, UCN can be stored for up to roughly 880 seconds (the $\beta$ decay lifetime) in a material bottle[6], and there exists a straightforward mechanism to polarize and transport UCN (without the restriction to straight guides).

At present the only available UCN source for a user community is located at the Institute Laue-Langevin (ILL), in Grenoble, France [11, 55, 57, 67]. The ILL UCN source is based on a population of neutrons thermalized in 20 liters of liquid.
deuterium. Neutrons are extracted vertically from the source and then a mechanical turbine is used to slow cold neutrons (CNs) or very cold neutrons (VCNs) down to ultracold neutrons (UCNs).

Recent source development projects have concentrated on an alternative to traditional sources to generate UCN: the superthermal process. The superthermal UCN source concept was first proposed using a superfluid $^4$He source by R. Golub and M. Pendlebury in 1975 [16,17,18,20, 21, 22]. The first experimental verification of the technique followed a few years later. From the detail balance principle, we know that if the energy between ground state and the excited state is $\Delta$, then the relationship of up-scattering and down-scattering will be

$$\sigma_{up} = \sigma_{down} \frac{E_{UCN} + \Delta}{E_{UCN}} \exp\left(-\frac{\Delta}{kT}\right).$$  \hspace{1cm} (1.2)

UCN production occurs when incident cold neutrons lose almost all their energy by the creation of a phonon in the He bath and become UCN. The reverse process (up-scattering) is suppressed by maintaining the moderator at low temperatures. UCN can therefore accumulate through this unbalanced process. The key here is that the neutrons never come into thermal equilibrium. The up-scattering rate is too low. In the case of superfluid $^4$He, this results in an experimentally verified increase in the population of UCN relative to neutrons in thermal equilibrium with the $^4$He moderator.

![Figure 1.2.1 UCN Generation](image-url)
Only a few materials have been carefully studied as UCN converters. Solid deuterium has proven to be a good candidate for a superthermal UCN source as well [26, 48, 53, 54, 59]. Ultimately, the UCN density in the source ($\rho$) is determined by a balance between the UCN production process ($P$) and destruction rates in the solid deuterium (SD2). If the UCN lifetime in SD$_2$ is represented by $\tau$, then:

$$\rho = P \cdot \tau . \quad (1.3)$$

There are several processes that result in UCN losses inside solid deuterium: phonon up-scattering, up-scattering from Para deuterium molecules, absorption by the deuterium, and absorption by hydrogen impurities. All of these effects will limit UCN density in SD$_2$, with the total loss rate, $1/\tau$, given by:

$$\frac{1}{\tau} = \frac{1}{\tau_{abs-D}} + \frac{1}{\tau_{abs-H}} + \frac{1}{\tau_{up-phonon}} + \frac{1}{\tau_{up-paraD_2}} \quad (1.4)$$

The UCN lifetime in solid deuterium has been measured at LANL by UCNA collaboration at Los Alamos National Lab. Since UCN lifetime in pure para-D2 solids is about 1.5msec [34], we want to keep the Para D2 fraction as small as possible. From an earlier study, we know that UCN lifetime is about 25 ms for a 2% Para fraction solid deuterium with 0.2% HD at about 5 K [38].
Chapter 2

UCN Production of Solid Deuterium

Fundamental neutron physics measurements using UCN are typically statistics limited due to the low UCN flux. To improve UCN production rate in UCN source is thus a critical issue for the UCN researcher. Presently in both sources constructed in the U.S., solid deuterium is being utilized as the UCN converter at both LANL and NCSU. In this chapter we will discuss the methods of evaluating solid deuterium UCN production.

2.1 Introduction to CN and UCN Production

To model the UCN production, we first use either MCNPX 2.4 (Monte Carlo N-particle, high energy simulation code) [65] or MCNP 5.0 (Monte Carlo N-Particle simulation code) [58] to calculate the cold neutron flux averaged over the SD$_2$ converter volume.

MCNPX is a Monte Carlo particle transport program coupled with the high energy proton-neutron cross sections, and is suitable for simulating a spallation neutron source. MCNP is the more commonly used neutron particle transport code, used for neutron, photon, electron, or coupled neutron/photon/electron transport.

For our application, we used rebuilt S($\alpha$,$\beta$) scattering kernels for room temperature Al and Be, and cryogenic scattering kernels for CH$_2$ at 77k and 4k [25], and solid methane at 22k and solid deuterium at 5 K [25]. The energy range was

6
expanded from the lower range of 1meV to 1μeV. To study VCN production, we also modified the MCNP code to make the neutron energy range even lower: down to $10^{-8}$ eV range. However, the reflection model in MCNP has to be updated in order to properly simulate VCN transport in the future.

We then calculated the neutron down-scattering cross section based on the incoherent approximation and various effective densities of states. The effects of molecular degrees of freedom were also incorporated. The molecular transition effect was treated with both one phonon [34] and multi phonon expansion treatment [35]. UCN energy are integrated up to 335 neV which is the Fermi-potential of a $^{58}$Ni surface.

The coherent inelastic scattering is estimated to be slightly larger (2% in current LANL case) than the incoherent scattering contribution.

Once we have calculated the UCN production rate, normalized to the proton beam, based on the simulated cold neutron flux and our down-scattering cross
section, it is then necessary to model the transport of UCN, a physically different problem [15, 41, 42]. Because MCNP is not appropriate for this purpose, we developed a customized Monte-Carlo transport code to simulate the UCN transport inside the solid deuterium and guide system. The reason we cannot use MCNP to simulate the UCN transport is that MCNP is a ray-tracing program and the effect of gravity, magnetic fields, non-specular scattering, and absorption losses of reflected neutrons have not been embedded properly in the current version. The trajectories of UCN are very different from tradition thermal neutron and cold neutron decay (see Figure 2.1.2). UCN transport resembles a ball bouncing through the guide tubes. We note also the MCNP’s energy range must be dramatically extended to properly simulate UCN transport.

Figure 2.1.2 LANL SD2 UCN Source (left) with a sample UCN trajectory (right)

2.2 UCN Cross Section Calculation

From Fermi’s golden rule, the neutron scattering partial differential equation can be expressed as [35]:

\[
\frac{1}{2\pi} \int d^2k \frac{\sigma(k)}{E} = \frac{\Delta E}{\hbar} \frac{N}{1 + e^{\Delta E/k_B T}}
\]
\[
\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{k} \left| \langle k' \lambda' | V(r) | k \lambda \rangle \right|^2 \delta(E - E' + E_h - E) \\
= \frac{k'}{k} \left| \langle n_f \left| \sum_i a_i e^{iQ \cdot R_i} \right| n_i \rangle \right|^2 \delta(E_f - E_i - \hbar \omega). \tag{2.1}
\]

Then

\[
\frac{d^2\sigma}{d\Omega dE_f} = \frac{1}{N} \frac{k'}{k} \sum_{n_f, n_i} P_n \sum_{i,j} a_i^* a_j \langle n_i | e^{iQ \cdot R_i} | n_f \rangle \langle n_f | e^{iQ \cdot R_j} | n_i \rangle \delta(E_f - E_i - \hbar \omega), \tag{2.2}
\]

where \(k\) and \(k'\) are the initial and final neutron momentum, \(Q\) is moment transfer, \(n_i\) and \(n_f\) are initial and final neutron states, \(i\) and \(j\) sum over lattice sites, \(N\) is the total number of target atoms, and \(a_i\) and \(a_j\) are scattering lengths. The scattering length is related to the interaction potential between a neutron and nuclei expressed, in the Born approximation, by (see Fig. 2.2.1)

\[
V(r) = \frac{2\pi \hbar^2}{M_n} \sum_i \{a_i \delta(r - R_i)\}, \tag{2.3}
\]

And we know

\[
|\langle V(r) \rangle|^2 = \sum_{i,j} a_i a_j e^{i\kappa(r - r_j)}. \tag{2.4}
\]

Figure 2.2.1 Neutron Scattering from Nuclei
We can rewrite Eq (2.4) as:

\[
\sum_{i,j} a_i a_j = |a_i|^2 + \sum_{i,j} \delta_{i,j} (|a_i|^2 - |a_j|^2) = a_{coh}^2 \sum_{i,j} e^{i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_i)} + a_{inc}^2 \sum_{j} e^{i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_i)} ,
\]

(2.5)

We can then express the scattering cross section into two distinct parts:

\[
\frac{d^2\sigma}{d\Omega dE_f} = \left( \frac{d^2\sigma}{d\Omega dE_f} \right)_{coh} + \left( \frac{d^2\sigma}{d\Omega dE_f} \right)_{inc} ,
\]

(2.6)

Where the coherent scattering cross section follows from the first term in Eq. 2.5 and the incoherent scattering cross section follows from the second term. They can be expressed by the scattering law following Van Hove’s treatment [44].

\[
\left( \frac{d^2\sigma}{d\Omega dE_f} \right)_{coh} = \frac{1}{N} \frac{k'}{k} \sum_{n_j, n_i} P_{n_i} a_{coh}^2 \sum_{i} \left| \langle n_f | e^{i\mathbf{Q} \cdot \mathbf{R}} | n_i \rangle \right|^2 \delta(E_f - E_i - \hbar \omega)
\]

\[
= a_{coh}^2 \frac{k'}{k} S_{coh}(Q,\omega) ,
\]

(2.7)

\[
\left( \frac{d^2\sigma}{d\Omega dE_f} \right)_{inc} = \frac{1}{N} \frac{k'}{k} a_{inc}^2 \sum_{n_j, n_i} P_{n_i} \sum_{i} \left| \langle n_f | e^{i\mathbf{Q} \cdot \mathbf{k}} | n_i \rangle \right|^2 \delta(E_f - E_i - \hbar \omega)
\]

\[
= a_{inc}^2 \frac{k'}{k} S_{inc}(Q,\omega) ,
\]

(2.8)

After the expansion, the coherent scattering cross section will be
\[
\frac{d^2 \sigma}{d\Omega dE_f} = \frac{\sigma_{coh}}{4\pi \ k} \frac{k^4 (2\pi)^3}{v_0} \exp \left\{ \left( \kappa \cdot \mu_0(0) \right)^2 \right\} 
\times \sum_s \sum_{\tau} \frac{(\kappa \cdot e_s)^2}{\omega_s^2} \left\{ \left( \langle n_s + 1 \rangle \times \delta(\omega - \omega_s) \delta(\kappa - q - \tau) \right) + \left[ \langle n_s \rangle \times \delta(\omega + \omega_s) \delta(\kappa + q - \tau) \right] \right\}, \tag{2.9}
\]

Where \( \mu_0(0) \) is the RMs displacement of a nuclei site from equilibrium, \( \omega_s \) is phonon normal modes, \( v_0 \) is the volume of the unit cell of the crystal. In Eq. 2.9, the terms proportional to \( \langle n_s + 1 \rangle \) involve in the creation of one phonon and the terms with \( \langle n_s \rangle \) involve in the annihilation of one phonon. Note coherent scattering follows energy conservation and moment conservation which lead to the identifications.

\[
E - E' = \hbar \omega_s \ ; \ k - k' = \tau \pm q . \tag{2.10}
\]

And

\[
\sum_j \left\{ \exp\{ -i\kappa \cdot R_j(0) \} \exp\{ -i\kappa \cdot R_j(t) \} \right\} = N \left\{ \exp\{ -i\kappa \cdot \mu_0(0) \} \exp\{ -i\kappa \cdot \mu_0(t) \} \right\} \tag{2.11}
\]

Also Eq. 2.9 can be expressed as [22]

\[
\frac{d^2 \sigma}{d\Omega dE_f} = \frac{k'}{k} a_{coh}^2 \frac{e^{2W(\kappa)}}{v_n - \frac{\partial \omega(q)}{\partial q}} \frac{\hbar}{2M} \sum_{s,q} \frac{|\kappa \cdot e_s|^2}{\omega_s(q)(e^{\frac{\hbar \omega_s(q)}{k_B T}} - 1)} , \tag{2.12}
\]

Where \( e^{-2W(\kappa)} \) is the Debye Waller factor, and in general, temperature dependent. \( e_s \) is polarization index.

For cubic structures, \( \left| \kappa \cdot e_s \right|_{ave}^2 = \frac{1}{3} \kappa^2 |e_s|^2 \). And the incoherent cross section will be
\[
\left( \frac{d^2 \sigma}{d\Omega dE} \right)_{\text{inc}} = \frac{\sigma_{\text{inc}}}{4\pi} k^I \left( \frac{1}{2M} \right) \exp \left\{ \left( \kappa \cdot \mu \right)_0 \right\}^2 \sum_s \frac{(\kappa \cdot e_s)^2}{\omega_s} \times \\
\left\{ \left[ \langle n_s + 1 \rangle \times \delta(\omega - \omega_s) \right] + \left[ \langle n_s \rangle \times \delta(\omega + \omega_s) \right] \right\} 
\] (2.13)

or

\[
\left( \frac{d^2 \sigma}{d\Omega dE_f} \right)_{\text{inc}} = \frac{k^I}{k} a_{\text{inc}} \sum_{n_f, n_i} \frac{\hbar}{2MN\omega(q)} e^{-2W(q)} |\kappa \cdot e_s|^2 \times \left\{ \frac{(n_s(q))}{\omega_s} \delta(\hbar \omega_{s,q} + \hbar \omega) \right\} \left\{ \langle n_s(q) + 1 \rangle \delta(\hbar \omega_{s,q} - \hbar \omega) \right\} 
\] (2.14)

It only follows the energy conservation;

\[
E - E^* = \hbar \omega_s 
\] (2.15)

\[
\left( \frac{d^2 \sigma}{d\Omega dE} \right)_{\text{inc} \pm 1} = \frac{\sigma_{\text{inc}}}{4\pi} k^I \left( \frac{3N}{2M} \right) \exp \left\{ \left( \kappa \cdot \mu \right)_0 \right\}^2 \frac{(\kappa \cdot e_s)^2}{\omega_s} Z(\omega) \left\{ \langle n_s + 1 \rangle \right\} 
\] (2.16)

Where \( Z(\omega) \) is the phonon density of states. The Eq. 2.14 can be expressed as

\[
\left( \frac{d^2 \sigma}{d\Omega dE_f} \right)_{\text{inc}} = \frac{4\pi a_{\text{inc}}^2}{k} \frac{m}{M} \int e^{-2W(k_f)} |e_s|^2 g(\omega)\sqrt{2m\omega / \hbar} \left( e^{\omega / \hbar k_f} - 1 \right) d\omega \] (2.17)

When considering about the solid molecular transition expansion, it will be

\[
\frac{d^2 \sigma}{d\Omega d\omega} = \sum_{J' = 0}^{J+1} S_{y,J} (2J'+1) |A_{y,J}|^2 C^2 (J'J;00) e^{i(E_J - E_{J'})/\hbar} \times \\
\left\{ \delta(\omega) + \left( \kappa \cdot \mu \kappa \cdot \mu(t) \right) + O(\kappa^4) \right\} 
\] (2.18)
2.3 UCN Production Calculation

If we express the cold neutron spectrum as \( \phi(E) = \frac{d\phi}{dE} \) then the spectrum for UCN produced by CN down-scattering \( S(E') \) is

\[
S(E') = N \int_{CN} \sigma(E \to E') \phi(E) dE
\]

(2.19)

Where \( \sigma(E \to E') = \frac{d\sigma}{dE'} \). Bottled UCN will have energies from zero to the maximum surface Fermi potential in the system, \( E_0' \). The characteristic dependence of the UCN energy can be read directly from the production cross-section as \( k^2 dk \) or \( \sqrt{E} dE \). Defining the total UCN production rule as

\[
S_0 = \int_{0}^{E_0'} S(E') dE'
\]

We see that

\[
S_0 = \int_{0}^{E_0'} \left[ N \int_{CN} \sigma(E \to E') \phi(E) dE \right] dE'
\]

\[
= N \int_{CN} \left[ \int_{0}^{E_0'} \sigma(E \to E') dE' \right] \phi(E) dE
\]

\[
= N \int_{CN} \sigma(E) \phi(E) dE
\]

\[
= N \langle \sigma(E) \rangle \phi_0
\]

(2.20)

Thus, the total UCN down scattering cross section will be
\[
\sigma(E) = \int_{0}^{E_{\text{CN}}} \sigma(E \rightarrow E')dE'
\] (2.21)

Inserting this definition into equation 2.20,

\[
\langle \sigma(E) \rangle = \frac{1}{\phi_0} \int \sigma(E)\phi(E)dE
\] (2.22)

where we use

\[
\phi_0 = \int \phi(E)dE
\] (2.23)

### 2.4 Solid Deuterium Crystal Lattice Dynamics and Coherent Inelastic Scattering Evaluation

The solid deuterium crystal has a hexagonal close-packed lattice structure. Each unit cell has two deuterium atoms. There are two sets of atoms which form the whole lattice. The phonon dispersion curve of solid deuterium at 5k was measured by M. Nielsen and his colleagues [43] using a neutron inelastic scattering technique. The measured data had been fitted by a third-nearest-neighbor Born-Von Karman theoretical model.

We reproduced their fitted phonon dispersion curve and also calculated the phonon density of states based on the model. From the dispersion curve, we can find the intersection points which indicate the contributions to the coherent inelastic scattering cross-section. Also from the phonon density of states, we can calculate the incoherent inelastic scattering cross-section [63].
As we know, the total cross-section can be expressed as sum of coherent and incoherent parts [44].

\[
\sigma = 4\pi \langle a \rangle^2 S_c + 4\pi \left[ \langle a^2 \rangle - \langle a \rangle^2 \right] S_i
\]  

(2.24)

If we define \( \delta S = S_c - S_i \)

Then

\[
\sigma = 4\pi \langle a^2 \rangle S_i + 4\pi \langle a \rangle^2 \delta S
\]  

(2.25)

Assuming the second term of Eqn. 2.25 is much smaller than the first term, then one can use the first term of Eqn. 2.25 for the approximated total cross-section; This is the widely used “incoherent approximation”. In fact, Placzek and Van Hove [44] evaluated the accuracy of the incoherent approximation for wave vectors (K) approaching zero. For cubic center crystals, the incoherent approximation gives roughly up to 20% error. To compare with our UCN production estimation using
incoherent approximation, we developed a numerical method[32] to evaluate the coherent inelastic scattering of 5 K SD$_2$ based on the phonon dispersion curve we reproduced. For incident neutron energies up to 10 meV and a UCN cutoff energy 335 neV, the coherent inelastic cross section is about 2% higher than that provided by the incoherent approximation.

Figure 2.4.2 Phonon Dispersion Curve of SD$_2$ with Free Neutron Dispersion Curve

The scattering law for one phonon interactions is:

\[
S^\pm (\vec{k}, \omega) = \frac{1}{2M_s} e^{-2W(\vec{k})} (2\pi)^3 \sum_{j=1,2,3} \sum_{q, \tau} \frac{|\vec{k} \cdot \sigma_j(q)|^2}{\omega_j(q)} (n + \frac{1}{2} \pm \frac{1}{2}) \delta(h\omega_{q, \tau} \mp h\omega) \delta^3(q \mp \vec{k} - \vec{\tau}), \quad (2.26)
\]

taken from Lovesey [35].

Figure 2.4.3 $S(\kappa, \omega)$ Used for SD$_2$ Coherent Inelastic Cross Section Calculation
The total scattering cross-section can be calculated from a set of $S(\kappa, \omega)$ tables, as shown in Eqn. 2.27. The coherent down-scattering cross-section is depicted in Fig. 2.4.5.

$$
\sigma_{\text{down}}^{\text{tot}}(E_i) = 2\pi b_{\text{coh}}^2 \frac{\hbar^2}{2mE_i} \sum_i \Delta \omega_i \sum_n \Delta k_n k_n S(k_n, \Delta \omega_i), \quad (2.27)
$$
2.5 Multiple Phonon Effect

The down-scattering rate can be calculated by using a multiple phonon expansion as well [35]. For our UCN production, the multiple phonon contribution is not important to incident neutron energies lower than 10 meV.

\[
\left( \frac{d^2 \sigma}{d\Omega dE} \right)_{\text{multiple-phonon}} = \frac{\sigma}{4\pi} \frac{k'}{k} \left( \frac{3N}{2M} \right) \exp \left\{ -2W(k) \right\} \left[ \frac{1}{\hbar \Delta} \exp \left\{ \frac{\omega}{\Delta^2 \gamma(0)} \right\} F(x, y) \right]\]

\[
x = \frac{\omega}{\Delta}; \quad (2.29)
\]

\[
y = 2W \exp \left\{ \frac{-1}{2\Delta^2 \gamma(0)} \right\} \quad (2.29)
\]

\[
F(x, y) = \sum_{p=2}^{\infty} \frac{1}{p!(2\pi \rho)^{1/2}} y^p \exp\left( -\frac{x^2}{2p} \right) \quad (2.30)
\]

Figure 2.5.1 Neutron Down-scattering Cross Section with Multiple Phonon Expansion
Chapter 3

Monte-Carlo Simulation for UCN Transport

3.1 Introduction to Neutron Transport by the Neutron Guide System

In a traditional, thermal or cold neutron facility, the details of the neutron play a critical role in determining the useful neutron flux for neutron scattering experiments. With this in mind, specialized tubes are optimized to transfer thermal or cold neutrons from the neutron source to an experimental facility 10 or more meters away. They can be curved to reduce gamma and fast neutron backgrounds. The guide system transmission efficiency is determined by the properties of the surfaces of guides, including surface roughness, material potential, incoherent up-scattering, and absorption in the surface layers of the guides. For thermal and cold neutrons, the reflection angles are very small, making even few mrad deviations of the neutron guides important. A larger angle will result in a large loss rate. Also only those materials with relatively high surface potentials are typically used for neutron guide systems, for example Be, Ni, $^{58}\text{Ni}$, diamond-like-carbon and super-mirrors.

On the other hand, UCN have very low energies. They are totally reflected for any angle of incidence for some surface materials, making highly curved guides and neutron material bottle geometries possible. Although total internal reflection does permit some flexibility in guide design, the UCNA experiment, for example, has some requirements which are not typical in CN guides systems. For example, the depolarization rate is below $3 \times 10^{-6}$ per bounce. The UCN depolarization rate should
be as low as possible to ensure the smallest possible systematic errors in the polarized beta-decay measurement.

For the UCNA experiment in its earliest phase, the important issue is “do we have adequate UCN transport to the beta-decay spectrometer?” This problem led us to try to develop a UCN transport code for our UCN guide system.

3.2 Introduction to UCN Transport

The UCN loss and reflection rate from a guide surface can be determined by solving the Schrödinger equation with proper boundary conditions, using an approximate model for the effective potential due to the material surface. Unfortunately guide surfaces are not ideal or locally flat. The guide materials absorb neutrons, they may contain contaminate, coating thicknesses may vary and the surface may be rough. The typical approach to this problem in simulations is to characterize the guide surface as a series of layers (see the examples R.Golub et al [22, 56]).

Neutrons can be reflected from the material surface, but the guide surface is not an ideal plane. Roughness caused by irregular deviations from an ideal smooth surface is described by the autocorrelation function. The loss rate and reflection rate are modeled by solving the surface scattering problem with the proper boundary conditions. UCN transportation simulations will finally give the transmission rate of UCN flux in the various guides systems.

3.3 UCN Guides

We use commercial quartz tubing as the “substrate” for our UCN guides. The average roughness is smaller than 1 nm over 1×1 um areas. Internal surfaces of these guides are coated with Diamond-Like-Carbon. A pulsed laser deposition (PLD)
technique was developed by other member of the UCNA collaboration [36, 69] to produce essentially hydrogen-free, very dense carbon coatings on cylindrical guide surfaces. The Fermi potential of the surface material is determined from the scattering length and number density of the surface material. For DLC coated guides, the Fermi potential is about 260 neV according to reflectometry measurements [36]. Variations in the Fermi potential are due to variations in the density of carbon and the hydrogen contamination. The specularity of the DLC guides is roughly 99.3%, and the loss per bounce is below 10E-4 as determined from the measurements on the prototype guides at ILL 2001 and 2002. One advantage of DLC guides for our UCNA project is that neutron depolarization rates on the DLC coating are very small. We also made use of some $^{58}$Ni/Mo coated guides which have a Fermi potential of about 330neV, specularity 97.5% and loss per bounce about 0.002 [26,62].

Figure 3.3.1 DLC Coated UCN Guide

3.4 UCN Reflection Models

Many aspects of the UCN guide quality will determine the UCN transport efficiency. The coating and surface smoothness are the most important parts. UCN
guide coating properties, which include coating material and coating thickness, will affect the UCN reflection rate. Surface smoothness will determine specular and nonspecular scattering.

1) Fermi potential:

The Fermi potential is determined by the number density and the scattering length of surface material:

\[
V = \frac{2\pi h^2}{m} Na, \quad (4.1)
\]

Where \( N \) is the number density of the surface material, \( m \) is the mass of the neutron and “a” is scattering length. For “real” DLC coatings, the average scattering length \( a_i \) could be smaller than that for a pure Diamond-Like-Carbon coating layer because of hydrogen contamination (hydrogen has negative scattering length), or because the Diamond Like Carbon number density might be lower than expected. We expect natural graphite’s density to be about 2.2g/cc, diamond to be about 3.2g/cc and DLC to be about 3g/cc. If we use 3g/cc then the expected Fermi potential will be 270 neV. However measurements data indicated that UCN spectra with much lower cut off energy (close to 100 neV) were surviving the UCN transport system in 2005. This brought to our attention another important factor: the coating thickness.

2) Coating thickness:

Our typical approach was to use Golub’s treatment [22] of a neutron wave interacting with a potential barrier with semi-infinite thickness, and to incorporate absorption into the reflection probability.
Following this prescription, we solve the Schrödinger equation:

\[ \varphi(x) = \begin{cases} e^{ikx} + \text{Re}^{-ikx}, & (x < 0) \\ Te^{ikx}, & (x > 0) \end{cases} \]  \hspace{1cm} (4.2)

Which results in a reflection index R:

\[ R = \frac{k - k'}{k + k'} = \frac{(E - V)^{1/2} - (E' - V)^{1/2}}{(E - V)^{1/2} + (E' - V)^{1/2}} \, . \]  \hspace{1cm} (4.3)

For real surfaces, we include potential to model UCN absorption

\[ U = V - iW = \frac{2\pi\hbar^2}{m} N(a - a_i) \, . \]  \hspace{1cm} (4.4)

Where \( a_i = \frac{\sigma_i k}{4\pi} \) represent the absorption and inelastic coherent scattering. The resultant reflection rate is:

\[ |R|^2 = 1 - 2 f \left( \frac{E}{V - E} \right)^{1/2} \, ; \quad f = \frac{W}{V} = \frac{\sigma_i k}{4\pi a} = \frac{\sigma_i}{2a\lambda} \, . \]  \hspace{1cm} (4.5)

However, in our case, some evidence indicates that our UCN guides DLC coating was too thin to be accurately modeled using semi-infinite barrier. Then it results a more realistic model of the surface potential in Figure 3.4.1. A thin DLC layer is depicted situated above a quartz substrate, making a two potential barriers problem.
The potential function is

\[ V(x) = \begin{cases} V_1, & (0 < x < a) \\ V_2, & (x > a) \end{cases} \]  \hspace{1cm} (4.6)

For \( V_2 < E < V_1 \), the wave function is:

\[ \varphi(x) = \begin{cases} e^{ikx} + \text{Re}^{-ikx}, & (x < 0) \\ Te^{ikx}, & (x > a) \end{cases} \]  \hspace{1cm} (4.7)

And inside the surface layer, the wave function will be \( \varphi(x) = Ae^{\kappa x} + Be^{-\kappa x}, (0 < x < a) \)

The boundary conditions for the front surface (\( x=0 \)) will be

\[ 1 + R = A + B \]
\[ \frac{ik}{\kappa} (1 - R) = A - B \]  \hspace{1cm} (4.8)

and boundary conditions for the back surface (\( x=a \)) are:
\[ Ae^{ikx} + Be^{-ikx} = Te^{ika} \]
\[ Ae^{ikx} - Be^{-ikx} = \frac{ik}{\kappa} Te^{ika} \quad (4.9) \]

② For \( E < V_2 < V_1 \) case, the wave function is:

\[ \varphi(x) = \begin{cases} e^{ikx} + \text{Re}^{-ikx}, & (x < 0) \\ Te^{ikx}, & (x > a) \end{cases} \quad (4.10) \]

The calculated reflection curve is shown below:

![Graph](image)

Figure 3.4.2 Thick DLC Coating Reflection Result

Figure 3.4.2 is reflection coefficient for a 100 nm DLC coating vs. neutron energy. Figure 3.4.3 is a plot of 10 the reflection coefficient for a 10 nm DLC coating reflection function vs. neutron energy.
3.5 UCN Specular and Non-Specular Scattering on Material Surfaces

Specular and non-specular scattering on the guide surface is discussed below. Specular scattering is just like light reflecting from a perfectly flat mirror. Nonspecular scattering is more complicated. It depends on the details of the roughness of a surface. A. Steyerl gives a treatment for neutron reflection on the micro-roughness of the surface. The deviation from an ideal mirror (specular scattering) surface is described using correlation function [56]:

\[
F(\delta) = \langle \xi(\rho)\tilde{\xi}(\rho - \delta) \rangle = \sigma^2 \exp(-\delta^2 / 2w^2)
\]

(3.1)
where $\sigma = \left\langle \varepsilon^2 \right\rangle^{1/2}$ is the mean square amplitude and $w$ is the correlation length for the roughness. The non-specular scattering probability can be expressed as:

$$I_{ns}(\theta_f, \phi_f) = \frac{3}{2\pi} G \cos \theta_i \cos^2 \theta_f \exp[-w^2 k^2 \left( \sin^2 \theta_i + \sin^2 \theta_f - 2 \sin \theta_i \sin \theta_f \cos \phi \right) / 2]$$  \hspace{1cm} (3.2)

When $k \sigma \ll 1$, the non-specular scattering probability $P$ can be approximately expressed as:

$$I_{ns}(\theta_f, \phi_f) = \frac{3}{2\pi} G \cos \theta_i \cos^2 \theta_f$$  \hspace{1cm} (3.3)

Since $P_{ns}(\theta_f) = \int I_{ns}(\theta_f, \phi_f) d\Omega_f$, from (3.3), we have

$$P_{ns}(\theta_i) = G \cos \theta_i$$  \hspace{1cm} (3.4)

This result indicates that non-specular scattering possibility depends upon the angle of incident wave to the surface normal $\cos(\theta)$, and outgoing UCN has a $\cos^2 \theta$ weighted distribution. This distribution can be sampled using Monte-Carlo methods to implement the non-specular scattering in collisions with an imperfect surface.
When $k_o \sigma >> 1$, all the nonspecular scatterings deviate from specular scattering by only very small angles. It roughly in a cone surrounding the outgoing specular vector.

Given that the angle between the incident neutron and surface normal is roughly equal to the angle of outgoing neutron direction and normal surface, the expression can be simplified. The non-specular scattering possibility vs. the theta and phi angles is shown in figure 3.5.3.
3.6 UCN Interaction with Magnetic Field

When UCNs pass through a magnetic field, they will be polarized. Those UCNs with spin anti-parallel to the B field will penetrate the potential barrier without being hindered (figure 3.6.1). UCNs with spin parallel to the B field will be filtered out if their kinetic energy is smaller than the potential barrier.

In our simulation of the UCN transport in a magnetic field, we incorporate magnetic forces on the UCN due to their interaction.

\[
F = -\nabla U = \nabla (u \cdot \vec{B}) = (u \cdot \nabla) \vec{B} + u \times (\nabla \times \vec{B}) + (\vec{B} \cdot \nabla)u + \vec{B} \times (\nabla \times u) \tag{4.11}
\]
The $(\vec{B} \cdot \vec{\nabla})u$ and $\vec{B} \times (\vec{\nabla} \times u)$ terms will be zero.

And $\vec{\nabla} \times \vec{B} = \vec{J} + \frac{\partial \vec{E}}{\partial t} = 0$. \hspace{1cm} (4.12)

So $\vec{F} = (u \cdot \vec{\nabla})\vec{B} = \frac{\gamma u_B}{|\vec{B}|} (\vec{B} \cdot \vec{\nabla})\vec{B}$; \hspace{1cm} (4.13) $\frac{dy}{dt} = V_y; \frac{dx}{dt} = V_x; \frac{dz}{dt} = V_z$ \hspace{1cm} (4.14)

Where $u_B$ is the nuclear Bohr magneton, and $\gamma$ is the gyromagnetic ratio.

\[
\frac{dV_y}{dt} = a_y = \frac{u_N}{m_N |\vec{B}|} (\vec{B}_x \frac{\partial B_y}{\partial x} + \vec{B}_y \frac{\partial B_y}{\partial y} + \vec{B}_z \frac{\partial B_y}{\partial z} - 9.8
\]

\[
\frac{dV_x}{dt} = a_x = \frac{u_N}{m_N |\vec{B}|} (\vec{B}_x \frac{\partial B_z}{\partial x} + \vec{B}_y \frac{\partial B_z}{\partial y} + \vec{B}_z \frac{\partial B_z}{\partial z})
\]

\[
\frac{dV_z}{dt} = a_z = \frac{u_N}{m_N |\vec{B}|} (\vec{B}_x \frac{\partial B_z}{\partial x} + \vec{B}_y \frac{\partial B_z}{\partial y} + \vec{B}_z \frac{\partial B_z}{\partial z})
\]

Figure 3.6.1 UCN Polarization Effect
3.7 UCN Transport Code

In order to better understand the UCN transport, we developed a Monte-Carlo UCN transport code. The features of the UCN transport code are listed below.

1) Each step of neutron movement is taken using Runge-Kutta numerical integration of equation of motion.

2) Gravity and magnetic fields have been included in the code.

3) The wall collision model has been characterized by the wall’s neutron losses (loss per bounce is average probability that UCN will be absorbed or upscattered during a collision), specular and non-specular reflection (specularity is the average probability of a mirror-like reflection). When the correlation length of the reflecting surface is large and the incident neutron energy is high, the nonspecular scattering is within a small solid angle around the outgoing direction. Otherwise it results in transport similar to diffusion. Note: Among all our UCN transport simulations, the only cases which examined different models of non-specular scattering effect were in the ILL depolarization measurement analysis (chapter 6).

4) Spin dynamics (depolarization on surface and spin flipping effect by though RF spin flipper) are included in the code for polarized neutrons.

5) The UCN transport inside the solid deuterium has been simulated by using incoherent elastic scattering, UCN absorption of SD2, and boost on the SD2 surface.
6) Other features, for example, mechanical flapper valve and the Al vacuum-isolation foil have been implemented as well.
Chapter 4

UCN Source at Los Alamos National Laboratory

From 2004 to 2006, we conducted a series of measurements to test the LANL UCN source performance. The measured UCN flux, however, did not match our design expectations [73]. After carefully comparing and cross-checking the calculations with our measurements which included cold neutron and UCN production, UCN transport and resultant UCN velocity distributions, we identified a set of issues with the current version UCN source. In this chapter, we give a detailed description of LANL UCN source, and a comprehensive analysis of both simulation results and measurement results. We will focus on the trouble-shooting of the UCN source performance and then finally conclude with our suggested improvements to the source at the end of 2005.

4.1 Introduction of LANL UCN Source

Los Alamos National Laboratory's UCN source relied on the spallation process to produce its primary neutron flux. Greater than roughly 100 MeV collisions between the incident particle (protons, neutrons etc.) and target nucleus has a “cascade effect”, resulting highly excited nuclei. The excited nuclei then relax by emitting neutrons in a process termed “evaporation”. This process can also be combined with fission.

For UCN source operation, we applied the LANCE, 800MeV proton beam [31] to our tungsten target. The resulting spallation neutrons were moderated by Be and Graphite surrounding cold polyethylene moderators. Thermal neutrons lose even
more energy and become cold neutrons (CN) by passing through a cold polyethylene moderator. Finally, UCNs are generated by the CN flux through a single down-scattering process.

The produced UCNs are guided up and out of the source chamber through a valve (called the flapper valve) and into a vertical guide section roughly 1 meter long. The UCNs then exit through an aperture at the top of the vertical guide into a horizontal guide system.

![Figure 4.1.1 UCNA Experiment Setup (top layer of source shielding removed)](image)

After that, the UCNs pass an "s"-shaped guide section with two 45-degree bends to reduce the backgrounds. The UCNs leave the biological shield; pass through a gate valve and a 7T pre-polarized magnet (PPM) which has an Al foil inside to separate the internal source vacuum and the instrument vacuum outside. As discussed in Chapter 1, UCNs exiting the 7T field region are highly polarized. They
then pass through a polarizer/spin-flipper magnet which has a tailored 1T field region optimized for a spin-flipper (with 5G RF fields) situated after the polarizing field. The UCNs then flow through a $3.5 \times 5$ cm guide with a rectangular cross-section and into a decay spectrometer (which is a 1 Tesla superconducting magnet with beta detectors located at the ends). The neutron beta-asymmetry will be measured inside the spectrometer [64, 70, 71]. (see Appendix A)

Figure 4.1.2 UCNA Experiment Cooling System

The solid deuterium UCN source cryostat and the three magnets will be cooled using liquid Helium. A closed Helium recycling system is used where returned cold Helium gas is compressed by one of three compressors and re-liquefied by a LN$_2$ – cooled Linde 1630 liquefier. Excess liquid Helium accumulates in a 4000 liter storage Dewar.

The deuterium gas handling system is used to purify and convert D$_2$ gas from the Para state (total nuclear spin of molecule $I=1$) to the Ortho state (total spin of
molecule I=0,2) [39, 40]. Purification is accomplished by allowing the D$_2$ gas to flow through a Palladium filter. Para-to-Ortho conversion is accomplished using FeO-OH gel held between 17.5 and 19 K [7, 32]. An additional Nitrogen trap can be used to pre-filter the D$_2$ gas to remove H$_2$O. After purification and conversion, the D$_2$ gas can be introduced to the Cryostat.

D$_2$ gas samples can be taken and measured by a simple Raman spectrometer to determine the Para/Ortho ratio of D$_2$ in the source. The average Para fraction of converted deuterium during the run circle is about 2% with about 0.2% hydrogen impurity, which provide a UCN lifetime about 25 ms in solid deuterium.
4.2 MCNPX Model of LANL UCN Source

For studying the neutronic performance of the UCNA source, we developed a MCNPX model of the spallation target system and the source chamber (Figure 4.2.1). The spallation target is a 2 cm diameter by 12cm long tungsten rod. A stainless steel chamber, filled with 250 PSI helium gas, is wrapped around the target. The UCN source chamber on top of the target is surrounded by many Be and graphite blocks in a moderator box. Be and graphite are both good moderators and reflectors and can be used to trap more thermal neutron flux near the cold moderator.

![Figure 4.2.1 MCNPX Model of LANL UCN Source](image)

Low temperature polyethylene beads serve as the cold neutron moderator. The beads are contained in a He vapor-cooled cup-shaped container situated around our D$_2$ UCN converter. The beads themselves are made of high density (0.92 g/cc)
polyethylene and are 1µm in diameter. They occupy a volume with wall thickness 1.1 cm and bottom thickness 0.6 cm. Cold He gas passes through the beads to produce typical operating temperatures between 20 and 60 K. The SD$_2$ is held in a 19.5 cm diameter, about 2 liters capacity aluminum chamber below a thermal break. A mechanical flapper valve coupled to a nominally 3” vertical guide is placed just above the SD$_2$.

Figure 4.2.2 Proton Radiographic Image (color scale is tied to number of proton’s in region)

The target system’s proton mesh tally and neutron mesh tally contour plots are shown in Fig. 4.2.2 and Fig. 4.2.4. The neutron generation rate per proton is about 11 neutrons per proton. Most thermal neutrons with energies from 10 meV to 0.625 eV are located at the bottom of a Tungsten target. But those neutrons with energies from 0~10 meV have their highest densities below the target and inside the converter chamber. It is very important to keep the cold neutron flux high inside of the UCN converter.
Figure 4.2.3 Neutron (0~10meV) Radiographic Image (color scale represents number of neutrons in region)

Figure 4.2.4 Neutron (10~625meV) Radiographic Image (color scale represents number of neutrons in region)
4.3 CN and VCN Benchmark Measurement

A cold neutron flux measurement to benchmark our MCNPX simulation was performed (Figure 4.3.1). We put a $^3$He detector on the top of shielding plug of the source. Neutrons in the proper solid angle passed first though an aluminum window between the vacuum source chamber and a collimator tube. The detector is situated just above the collimator. Its estimated detecting efficiency for thermal neutrons is close to 1.

![Figure 4.3.1 Cold Neutron Flux Measurement Model](image)

To avoid saturating our data acquisition system (DAQ), we pre-scaled the CN events by a factor of 10. The measurement and simulation results are shown in Fig. 4.3.2. In our simulation, we used both 1.2 liter and 2 liter volumes SD$_2$ with a 77 k polyethylene scattering kernel. The experimental SD$_2$ temperature was monitored by a couple of temperature sensors outside the converter chamber, and was between 4 and 20 K. The polyethylene was at about 150 K for this measurement. The simulated cold neutron flux was averaged over time in 1 ms bins from 1msec to 10
ms. The simulated total flux was $5.3 \times 10^4 \text{ CN/uC}$, higher than the measured CN flux by about a factor of 1.6. The Measured CN flux for 1200cc SD$_2$ was about $3.3 \times 10^4 \text{ CN/uC}$.

Figure 4.3.2 Comparison of Cold Neutron Measurement and Simulation Results

There are two possible explanations for the discrepancy between the measured cold neutron flux result and our simulations. One is that the collimator tube is slightly bent, attenuating the transmitted CN flux. The other is that the proton beam may be somewhat larger than the target, reducing the normalized CN production per incident proton.

Figure 4.3.3 Bend Collimator
A VCN flux measurement was also conducted last year. We placed a $^3$He MWPC detector inside the source chamber about 1.6 meters above the SD$_2$ surface. The MWPC was designed with an Al foil for the entrance window and was divided into a top and bottom chamber by Ni foil. UCN could penetrate the Al foil and be counted in the lower compartment of the MWPC, but could not penetrate to the upper compartment. In the upper compartment, only VCN and CN were counted. From the measurement results of the empty source and the source filled with SD$_2$, we can extract the VCN flux which is due to SD$_2$ down-scattering. The counts before 10 msec, actually much larger, saturated the internal detector’s preamps. The counts after 0.2 second were dominated by fast neutron’s product by n, $\gamma$ interaction on Be in the source.

Figure 4.3.4 VCN Measurement Setup and Source Insert
Those neutrons detected between 0.01 second and 0.25 second can be identified as neutrons with velocities between about 10 and 200 m/s. These neutrons can not be bottled for any significant length of time. Using a transport simulation to provide the overall calibration between production rate and incident proton beam current, we deduce a production rate of 85 UCN/cc/uC (where the production is specifically per unit volume of SD$_2$). This can be compared to an incoherent approximation calculation of 107 UCN/cc/uC for the production rate.

![Figure 4.3.5 VCN Measurement Result](image)

The fast neutron flux, at times larger than about 0.2 seconds, decays with a multi-exponential due to the wide variety of radio-nuclides and is believed to be due to the n,$\gamma$ process on Be. A particularly strong component may be due to Al decays producing neutrons with lifetimes of about 200 seconds.
4.4 Proton Beam Effect

A potential source of reduced UCN production is poor production beam tunes. Since proton beam profiles are approximated Gaussians, and the FWHM is comparable to the current dimensions of the target, we did some simulations to identify the proton beam effective FWHM. The measurement setup is shown in figure 4.4.1.

![Proton Beam Scan](image)

Figure 4.4.1 Proton Beam Scan

Because the direction of a proton beam can be changed using magnetic field steering, we scanned the center of the proton beam across the target both in the X and Y directions and measured the CN flux using the CN detector mounted above the shielding plug. To interpret the scan results, we used the following information from LANSCE: each 4A current change in the magnetized steering magnets produces a 1.7mrad angle deflection of the proton beam, and the distance from the quads to the W target surface is about 10.33 meters. This implies about a 2.2cm/A deflection. We compared the measured off-center CN profiles with simulation using this calibration. The results are shown in figure 4.4.2. The proton beam is obviously asymmetric in shape, and the x direction is broader than y direction (this was consistently true).
Figure 4.4.2 Proton Beam Scan Profile

We also carried out a simulation using different Gaussian beam sizes and with scanning across the target. The actual edges of the beam profile are determined by the guide walls, the geometry of the moderator box, and by a series of apertures along the beam (which provide some scattering, but probably do not define the full beam geometry). We didn’t include the apertures or the beam diffuser in our model. The measurement and simulation results seem best matched by a profile with a Y-axis sigma between 0.75cm to 1 cm, and an X-axis profile with sigma is between 1 cm and 1.25 cm. We used a full Gaussian profile (as opposed to a “cookie cut” profile in which the tails of the Gaussian are removed). We expected that the cookie cut may be more accurate but it makes no more than a 20% decrease in the CN counts.
Comparing absolute neutron flux calculations with these simulated scanning results, the sigma 1 to 1.25 cm cold neutron flux of about $3.3 \times 10^4$ CN/cc/μC corresponds well to our estimated best fit beam profiles.
Figure 4.4.5 Absolute MCNP Simulation Data of Proton Beam Y Scan

Figure 4.4.5 Absolute MCNP Simulation Data of Proton Beam X Scan
To estimate the effect of the beam profile on the UCN production (per uC of beam), we calculated the production for a symmetrical Gaussian beam profile as a function of the Gaussian sigma. We used a SD$_2$ volume of 1200 cc at 5K and a cold neutron moderator composed of 77 K polyethylene with an effective cold neutron moderator density of 0.5 g/cc. Our results indicate a drop of over a factor of three from the ideal beam profile used in initial calculations of production from our target (sigma < 0.5) and our inferred profile (1 cm < sigma < 1.25 cm).

![Proton Beam Size Effect](image)

Figure 4.4.7 Proton Beam Size Effect

### 4.5 Polyethylene Beads Cold Neutron Moderator

#### 4.5.1 The Effective Poly Density

For the LANL UCN source, we used polyethylene as the cold neutron moderator. The effective density of the polyethylene (poly) is determined by the
beads packed into the cold neutron source chamber. We measured the net mass of poly beads poured in an 80ml container as 43 g, yielding a density of naturally-packed poly beads of about 0.5 g/cc. When the beads were close-packed, we expected slightly greater density of about 0.62 g/cc, roughly 2/3 of poly density in a particle bead 0.92 g/cc [66]. For the “as-built” source, we think a poly beads density of 0.5 g/cc is a more representative value, because although we shook the source often and attempted to push the poly beads into the source through the two access holes into the can, it was not possible to pack the beads much more densely than one can achieve by simply pouring and shaking.

![Figure 4.5.1 Poly Beads Density Effect](image)

Figure 4.5.1 Poly Beads Density Effect

For our current source, UCN production should be roughly 107 UCN/cc/µC (incoherent approximation with real phonon spectrum) using a SD$_2$ volume of 1200 cc, about a factor of 1.5 lower than with the high density poly moderator.
4.5.2 Poly Temperature Effects

To investigate the effect of the temperature of the polyethylene beads on our ultra-cold neutron production, we carried out simulations using a 5 k SD2 scattering kernel, with a 2000cc Solid Deuterium converter and using 4k and 77k poly scattering kernels. UCN production due to these two cases is shown in table 4.5.1. The effect of the poly temperature change was insignificant.

Simulation cases:
1) Poly temp. #1 (4K poly scattering kernel);
2) Poly temp. #2 (77K poly scattering kernel).

<table>
<thead>
<tr>
<th>UCN production (UCN/cc/uC)</th>
<th>Using Incoherent approximation with Debye phonon spectrum</th>
<th>Using Incoherent approximation with real phonon spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poly temp #1</td>
<td>158 ± 8</td>
<td>136 ± 6</td>
</tr>
<tr>
<td>Poly temp #2</td>
<td>149 ± 7</td>
<td>127 ± 6</td>
</tr>
</tbody>
</table>

Table 4.5.1

4.6 Source Modification and Improvement

To improve the source performance, we investigated different modifications of the source. For example, we tried simulating the insertion of a high-density poly shell inside the source with various shell wall thicknesses. We also tried putting a poly disk on the bottom of the source. For every configuration, we evaluated the gain using fixed SD$_2$ volume (to offset SD$_2$ thickness changes). The results show that using a 2 cm thick poly shell increases the UCN production by a factor of about two,
but the bottom disk will not provide a significant gain factor. These conclusions had been proven by a set of UCN transport measurements when we used the same guides system. The beam profile used was a 2D Gaussian with $\sigma = 1\text{cm}$ and a cut off at 2 cm. 77k scattering kernels were used for the poly beads.

Figure 4.6.1 Geometry for Scans of the Poly Insert (the wall thickness was varied while leaving the volume of $\text{SD}_2$ constant)

Figure 4.6.2 Geometry Used To Vary The Poly Thickness On The Bottom Of The Cryostat
Adding a cold poly wall inside of the source could increase the CN and UCN. However there are potential problems with a poly insert as well. The low Fermi potential of poly would cause significant losses due to absorption, and low surface specularity might reduce the probability that UCN can escape the source. So the Fermi potential was a critical issue and all poly elements were either encapsulated in S.S., coated with $^{58}$Ni or wrapped in metal foil.
Our simulations indicated that poly inserts on the bottom of the source do not seem to be effective in increasing the CN flux. Also, the presence of these bottom disks partially isolates the SD$_2$ from the bottom surface of the cryostat.

![Graph](image1)

**Figure 4.6.5 Results of A Scan Over The Wall Thickness of The Poly Insert**

![Graph](image2)

**Figure 4.6.6 Results of A Scan Over The Thickness of A Poly Layer On The Bottom of The Cryostat**
The optimum poly insert wall thickness was found to be about 2cm. This produces the best balance between the SD$_2$ thickness and increase in the CN flux. To continue our optimization process, we then fixed the poly wall insert thickness to 2 cm, and did a scan of the wall-height for the poly wall insert.

Figure 4.6.7 Poly Insert Height Scan

![Poly Insert Height Scan](image)

Figure 4.6.8 Poly Insert Height Scan Result

![Poly Insert Height Scan Result](image)
The poly wall height scan results show that a 25cm height of 2cm thickness poly wall is roughly optimal. Increasing the wall height provides no further improvement of the CN flux in the SD$_2$ volume.

We also investigated the idea of placing a warm poly layer around the source, under the W target, and between the W target and source bottom. Because low energy neutrons will be absorbed by the source chamber or the complicated inner structure of the source, putting a warm poly layer outside of the source did not increase the CN flux except when we placed a poly layer between the source and the target. This yielded a slight gain in UCN production. But this layer’s thickness will be limited by the space between source chamber and target. From these studies, it would seem that the only useful way to increase the polyethylene moderator effectiveness is through the wall insert within the cryostat.

Three modifications cases using a warm outer poly layer are listed below, results of these changes are shown in table 4.6.1.

1) Poly layer #1 (2 cm warm poly wall around the source);
2) Poly layer #2 (warm poly layer below the W target);
3) Poly layer #3 (warm poly layer between the W target and the source).
<table>
<thead>
<tr>
<th>UCN production (UCN/cc/uC)</th>
<th>Using Incoherent approximation with Debye spectrum phonon</th>
<th>Using Incoherent approximation with real spectrum phonon</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poly layer #1</td>
<td>129 ± 7</td>
<td>111 ± 6</td>
</tr>
<tr>
<td>Poly layer #2</td>
<td>121 ± 7</td>
<td>102 ± 6</td>
</tr>
<tr>
<td>Poly layer #3</td>
<td>159 ± 8</td>
<td>134 ± 6</td>
</tr>
</tbody>
</table>

Table 4.6.1

The Tungsten target modification:

A final possible modification of our source geometry involves increasing the target volume. Currently we use the WNR target design to avoid Category Three inventory limitations. For further source development, we need to provide more simulation results for various W target sizes and lengths.

Figure 4.6.10 Target Size Effect
Simulation cases (case 5, target #3 corresponds to unmodified case):

1) W target #1 (20 cm long, 2cm diameter W rod);
2) W target #2a (12 cm long, 4 \(\times\) 4 cm square rod);
3) W target #2b (12 cm long, 5 \(\times\) 5 cm square rod);
4) W target #2c (12 cm long, 2.8 \(\times\) 4 cm square rod);
5) W target #3a (12 cm long, 2cm diameter W rod);
6) W target #3b (12 cm long, 3cm diameter W rod);
7) W target #3c (12 cm long, 4cm diameter W rod).

<table>
<thead>
<tr>
<th>UCN production (UCN/cc/uC)</th>
<th>Using Incoherent approximation with Debye phonon spectrum</th>
<th>Using Incoherent approximation with real phonon spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>W target #1</td>
<td>125 ± 5</td>
<td>107 ± 4</td>
</tr>
<tr>
<td>W target #2a</td>
<td>243 ± 7</td>
<td>209 ± 6</td>
</tr>
<tr>
<td>W target #2b</td>
<td>241 ± 7</td>
<td>205 ± 6</td>
</tr>
<tr>
<td>W target #2c</td>
<td>248 ± 7</td>
<td>212 ± 6</td>
</tr>
<tr>
<td>W target #3a</td>
<td>125 ± 3</td>
<td>107 ± 3</td>
</tr>
<tr>
<td>W target #3b</td>
<td>224 ± 6</td>
<td>191 ± 5</td>
</tr>
<tr>
<td>W target #3c</td>
<td>236 ± 7</td>
<td>201 ± 5</td>
</tr>
</tbody>
</table>

Table 4.6.2

Conclusions:
Gathering all possible improvements (Fig.4.6.11), we produced an “optimized solution”. This included a 2cm cold poly wall insert and a 2cm warm poly flapper disk (thicker than 2 cm would not provide higher CN flux and also flapper need to be light), and a 2.54 cm by 4cm square W target. Then we got a UCN production of
482±12 UCN/cc/uC (incoherent approximation with real phonon spectrum), or
560±14 UCN/cc/uC (incoherent approximation with Debye phonon spectrum), which
is higher than the 2005 UCN production by the approximate a factor of 4.5.

Figure 4.6.11 UCN Source Optimization

4.7 A Re-evaluation of the Prototype UCN Source

We also re-evaluated the prototype source using both a Gaussian proton beam
profile and uniform beam profile. The W target for the prototype source was a 5 × 17
× 17cm block covered with a 4cm thick poly block at 77k. We used both about 1000
cc solid Deuterium (20cm height) and about 400 cc solid Deuterium (8cm height) in
the source, surrounded by a 77k high density polyethylene wall (Fig.4.7.1). UCN
production results are shown in table 4.7.1. As might be expected, for this larger
target the UCN production is not sensitive to the proton beam size. The simulation
result is reasonably close to measured data (466±92 UCN/cc/uC)[47]. Note: in this
case, we used the 0.92g/cc for poly blocks density, UCN cutoff energy 227neV.
<table>
<thead>
<tr>
<th>UCN production (UCN/cc/uC) of 1000cc SD2</th>
<th>Using Incoherent approximation with Debye spectrum phonon</th>
<th>Using Incoherent approximation with real spectrum phonon</th>
</tr>
</thead>
<tbody>
<tr>
<td>uniform beam</td>
<td>639 ± 14</td>
<td>631 ± 13</td>
</tr>
<tr>
<td>Gaussian beam</td>
<td>639 ± 14</td>
<td>629 ± 13</td>
</tr>
</tbody>
</table>

Table 4.7.1

<table>
<thead>
<tr>
<th>UCN production (UCN/cc/uC) of 400cc SD2</th>
<th>Using Incoherent approximation with Debye spectrum phonon</th>
<th>Using Incoherent approximation with real spectrum phonon</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform beam</td>
<td>901 ± 21</td>
<td>826 ± 19</td>
</tr>
<tr>
<td>Gaussian beam</td>
<td>882 ± 20</td>
<td>817 ± 19</td>
</tr>
</tbody>
</table>

Table 4.7.2

Figure 4.7.1 Prototype UCN Source
4.8 Other Possible Cold Neutron Moderator

There are two other moderator candidates which can be used instead of polyethylene beads as a cold neutron moderator. They are solid methane and liquid hydrogen. When used in the geometry depicted before, 20k solid methane may have a UCN production rate about a factor at least 1.6 higher than low density (0.5g/cc) polyethylene beads at 77k temperature, with a 1200cc solid deuterium (5 K) converter. A 19k, 75% Ortho- and 25% Para-hydrogen liquid moderator has a factor of 1.3 higher production rate under the same condition.

<table>
<thead>
<tr>
<th>UCN production</th>
<th>Using Incoherent approximation with Debye spectrum phonon</th>
<th>Using Incoherent approximation with real spectrum phonon</th>
</tr>
</thead>
<tbody>
<tr>
<td>77k Low density Poly</td>
<td>125 ± 3</td>
<td>107 ± 3</td>
</tr>
<tr>
<td>20k Solid methane</td>
<td>194 ± 6</td>
<td>175 ± 5</td>
</tr>
<tr>
<td>19k Liquid Hydrogen</td>
<td>153 ± 5</td>
<td>139 ± 5</td>
</tr>
</tbody>
</table>

Table 4.8.1

It should be pointed out that solid methane also has some radiation damage effects which might prevent its use in the LANL source. For the high radiation fields at the spallation target for the UCNA source, one must be very careful to choose a cold neutron moderator based not only on its neutronic performance, but also on its thermal properties and its stability after large radiation doses. The total cross-section of SD$_2$ and Polyethylene used by MCNP is shown in appendix C.
4.9 DLC Coating Thickness Tunneling Effects and UCN Transport in UCNA Experiment

One of the most important factors governing UCN transport is the UCN reflectivity of the surface. UCN transport measurements at LANL indicated very low transmission for our DLC guides and a lower cut-off in the energy spectrum from the output of our DLC coated guides system. This situation could stem from two sources: lower Fermi potential and thinner DLC coating.

In our current model, neutron waves reflected from two potential barriers: a 260neV barrier due to DLC and an 80neV barrier due to the quartz substrate. After solving the Schrödinger equation with appropriate boundary conditions, a 3D plot of the reflection vs. layer thickness and incident neutron energy is shown in figure 4.9.1.

![3D plot of UCN reflection vs. layer thickness and incident neutron energy](image1.png)

Figure 4.9.1 UCN reflection curves with various DLC coating thickness

If the DLC layer is thick enough, the reflection curve will drop just above 260neV, where there are some interference effects as the reflecting drops. The total length of our horizontal guides is about 6~12 meters long, and the average number of UCN
bounces will be of about 40~80 before they reach the decay trap. It is clear that if
the UCN reflectivity falls below 75%, UCN will have a very small probability of
reaching the end of the guide system and being detected.

For thinner coatings, there will be a tunneling effect. From the calculated results
of the thinner coating case, we can see that instead of a sharp drop above 260neV,
the reflection curve slowly drops above 80neV. UCN transmission results with the
tunneling effect are presented in the next section.

### 4.10 UCN Transport Measurement at LANL

To determine the UCN transport efficiency, we set up a transmission
measurement in 2005. A $^{3}$He UCN detector coupled to a vertical guide section was
connected to the horizontal UCN guide system just beyond the first gate valve. The
location of the detector is shown in Fig4.10.1 and the results are shown in figure
4.10.2. The UCN flux is normalized to each pulse.

![Figure 4.10.1 UCN Transport Measurement Setup](image)
To compare with our measurement results, we used the reflection model of section 4.9 (two layer model) in the UCN transport code. The DLC Fermi potential used is 260 neV. The source chamber vertical guide potential used is 330 neV (Ni58 coated S.S. guides), and the two 45 degree bends adapters’ (fabricated of polished stainless steel) had specularities of about 80%. The DLC coating thickness for the horizontal guides is independently fixed for each guide component. To better understand the UCN transport inside the SD$_2$, we added a “chevron” structure inside the source and set the incoherent elastic free path length to 8 cm. The UCN lifetime in the SD$_2$ is about 25ms, using the Raman spectrum results of 2% Para D$_2$ fraction and 0.2% H$_2$ impurity. The total transmission rate is about 1.2% with 100nm DLC coating and is about 0.32% with 10nm DLC coating. To get good agreement with the data, a DLC thickness of 30 nm is required, certainly not thick enough to efficiently transport UCN up to the 260 neV cut-off into our decay bottle. Therefore improvements in the DLC guide coating will be a critical issue in maximizing the available UCN flux.

Figure 4.10.2 Comparison of UCN Transport Measurement and Simulation Results
In the transport code, we set up tally detectors at different positions along the guide system. These surface detector tallies specify the UCN transmission at different locations based on the current guide geometry.

![Figure 4.10.3 UCN Transport Simulation Geometry Profile](image)

<table>
<thead>
<tr>
<th>Tally number</th>
<th>DLC coating thickness 20 nm</th>
<th>DLC coating thickness 30 nm</th>
<th>DLC coating thickness 40 nm</th>
<th>DLC coating thickness 60 nm</th>
<th>DLC coating thickness 100 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tally11</td>
<td>31.09±0.56 %</td>
<td>30.81±0.56 %</td>
<td>31.18±0.56 %</td>
<td>30.48±0.55 %</td>
<td>30.73±0.55 %</td>
</tr>
<tr>
<td>Y=0.05m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tally12</td>
<td>15.85±0.4 %</td>
<td>15.64±0.4 %</td>
<td>15.89±0.4 %</td>
<td>15.71±0.4 %</td>
<td>15.74±0.4 %</td>
</tr>
<tr>
<td>Y=0.13m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tally13</td>
<td>13.39±0.37 %</td>
<td>13.12±0.36 %</td>
<td>13.39±0.37 %</td>
<td>13.34±0.37 %</td>
<td>13.28±0.36 %</td>
</tr>
<tr>
<td>Y=0.94m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tally14</td>
<td>6.35±0.25 %</td>
<td>7.07±0.27 %</td>
<td>7.67±0.28 %</td>
<td>7.72±0.28 %</td>
<td>7.75±0.28 %</td>
</tr>
<tr>
<td>Z=0.3m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tally15</td>
<td>4.02±0.2 %</td>
<td>4.56±0.21 %</td>
<td>5.51±0.23 %</td>
<td>6.19±0.25 %</td>
<td>6.44±0.25 %</td>
</tr>
<tr>
<td>Z=2.2m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tally16</td>
<td>1.76±0.13 %</td>
<td>2.31±0.15 %</td>
<td>3.02±0.17 %</td>
<td>3.81±0.2 %</td>
<td>4.03±0.2 %</td>
</tr>
<tr>
<td>Z=3.3m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tally18</td>
<td>0.84±0.07 %</td>
<td>1.28±0.08 %</td>
<td>1.64±0.09 %</td>
<td>2.42±0.11 %</td>
<td>2.72±0.12 %</td>
</tr>
<tr>
<td>Z=6.2m</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 4.10.1 UCN Transport Simulation Results
Given problematic results with our DLC guides, we proposed to use high polished stainless steel tubes for the horizontal guides section for the 2006 run. The simulation result of this case is also shown in table 4.10.3.

The neutron flux vs. $\cos(\theta)$ and UCN energy plots are shown in Fig 4.10.4 and Fig 4.10.5. Theta is the angle between the neutron direction and the guide axis. The first plot indicates that the UCN flux has a very narrow forward peak with 100~150 neV UCN average energy at the end of guide system (first gate valve). This model is with a DLC thickness greater than 100 nm. The second simulation incorporated a 30 nm and yielded a much lower cut-off energy of about 50~80 neV in the end.

Figure 4.10.4 UCN Transport Simulation Beam Profile I
To establish the presence of a low energy cut-off in the UCN spectrum existing in our horizontal guides system, we also have a PPM B-field scan. The 7T magnetic field mapping is shown in Figure 4.10.7.
As we know, there was 20 mil thick Aluminum foil inside the PPM to separate the source vacuum from the experimental vacuum. In fact the primary function of the PPM is not to polarize UCN, but also to pull one spin state UCN through the Al window, roughly doubling the overall transmission.

The transmission rate of the foil can be expressed as $T$,

$$T = e^{-\Sigma v d / \cos(\theta)} = e^{-\beta d / \nu \cos(\theta)} = e^{-\beta d / v_\perp}$$ (4.16)

Where $V_\perp$ is the total cross-section of the Al foil. $d$ is the thickness of foil. $V_\perp$ is the perpendicular velocity. The UCN absorption cross-section of aluminum is about 130 barns at a velocity of 5 meters per second and 1/v dependent [23]. In our simulation, PPM transmission rate can be calculated by the ratio of tally19 ($z=7.95m$) over tally18 ($z=6.18m$) counts.

Figure 4.10.7 PPM Magnetic Field Scan
Figure 4.10.8 PPM Scan with the Original DLC Coating (thin coating) Quartz Horizontal Guide System

Figure 4.10.9 PPM Magnetic Field Scan with New S.S Horizontal Guide System

The first results show that a higher Magnetic field will push more UCN through the Al window. The magnetic field used here is 7T. The Al foil used is 4 mil thick; all
DLC Fermi potential is 262 neV. The second figure shows the PPM polarization effect.

To explore modifications to the UCN transport, we carried out simulations using the same geometric set up (with UW insert inside the source) and different horizontal guide systems. The 10 mil thick Al foil is used with a 7 T PPM field. The polished S.S. tubes' (with $^{58}$Ni coating thickness 150 nm) specularity is 97.5% (Serobrov guide) and the $^{58}$Ni Fermi potential used is 335 neV. Normal S.S tubes' surface specularity is 80% [24] and Fermi potential is 180 neV. (But this does not apply to 2006 studies guides of specularity larger than 99% [62].)

<table>
<thead>
<tr>
<th>Tally</th>
<th>DLC coating thickness 20 nm</th>
<th>S.S. tubes (specularity 80%)</th>
<th>DLC coating thickness 150 nm</th>
<th>Polished S.S. tubes with $^{58}$Ni coating thickness 150 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tally11 Y=0.05m</td>
<td>30.69±0.55 %</td>
<td>31.32±0.56 %</td>
<td>30.99±0.56 %</td>
<td>30.89±0.56 %</td>
</tr>
<tr>
<td>Tally12 Z=0.13m</td>
<td>15.52±0.39 %</td>
<td>16.01±0.40 %</td>
<td>15.81±0.40 %</td>
<td>15.93±0.40 %</td>
</tr>
<tr>
<td>Tally13 Y=0.94m</td>
<td>12.84±0.36 %</td>
<td>13.41±0.37 %</td>
<td>13.40±0.37 %</td>
<td>13.31±0.36 %</td>
</tr>
<tr>
<td>Tally14 Z=0.3m</td>
<td>6.06±0.25 %</td>
<td>7.95±0.28 %</td>
<td>7.79±0.28 %</td>
<td>6.74±0.26 %</td>
</tr>
<tr>
<td>Tally15 Z=2.2m</td>
<td>3.86±0.20 %</td>
<td>6.80±0.26 %</td>
<td>6.52±0.26 %</td>
<td>5.49±0.23 %</td>
</tr>
<tr>
<td>Tally16 Z=3.3m</td>
<td>1.72±0.13 %</td>
<td>4.41±0.21 %</td>
<td>4.40±0.21 %</td>
<td>3.27±0.18 %</td>
</tr>
<tr>
<td>Tally17 Z=4.3m</td>
<td>1.07±0.10 %</td>
<td>3.22±0.18 %</td>
<td>3.26±0.18 %</td>
<td>2.16±0.15 %</td>
</tr>
<tr>
<td>Tally18 Z=6.2m</td>
<td>0.93±0.096 %</td>
<td>3.04±0.17 %</td>
<td>3.14±0.18 %</td>
<td>2.06±0.14 %</td>
</tr>
<tr>
<td>Tally19 Z=7.4m</td>
<td>0.09±0.030 %</td>
<td>0.69±0.083 %</td>
<td>0.74±0.086 %</td>
<td>0.51±0.071 %</td>
</tr>
<tr>
<td>Tally20</td>
<td>0.06±0.025 %</td>
<td>0.615±0.079 %</td>
<td>0.645±0.081 %</td>
<td>0.48±0.069 %</td>
</tr>
</tbody>
</table>

Table 4.10.3
The absolute UCN flux can be also estimated by our analysis method. Assume the UCN production is 107 UCN/cc/uC and the SD$_2$ volume is about 1200 cc (the largest volume used in 2005). The simulated UCN transmission behind of the first gate valve was about 1.28% with a thin DLC coating quartz guide (30nm). So the total calculated UCN count at this location was about 1643 UCN/uC. The measured UCN flux last June with the elephant trunk detector was about 672 UCN/uC. Assuming a 75% transmission of 90 degree bend and UCN detector efficiency is 50%, then we have UCN count about 896 UCN /uC at first gate valve. In the PPM scan, the measured UCN count is about 293 UCN/uC behind the PPM with a 75% transmission of 90 degree bend and a 50% detector efficiency. Our simulation result (30nm DLC layer) was about 334 UCN/uC. This simulation used a 10 mil Al foil inside a 7 T PPM field. Note that the foil used in 2005 may be thicker than 10 mils [73]. And the DLC coating may be even thinner than 30 nm. So we roughly understand the 2005 LANL source production. Differences of transmission due to small gaps and other losses in guides system needs to be considered in future work.
Chapter 5

The North Carolina State University PULSTAR Reactor UCN Source

A UCN source has already been in the design and engineering phase for about six years at NCState University. The UCN production rate in a SD\(_2\) converter was evaluated by combining an MCNP model of the CN flux and the calculated down-scattering cross section in SD\(_2\). We note that the cold neutron flux is strongly dependent on the geometry of the cold source and the materials of the cold neutron moderator. Simulation results have permitted us to optimize the source neutronic performance and to evaluate the nuclear heat load, a critical input in the design of the source cryogenic cooling system. Transport of the resultant UCN flux has also been simulated using a Monte Carlo UCN transport code (see Chapter 3).

To benchmark the MCNP simulation results, we also conducted an absolute thermal neutron flux measurement in the reactor thermal column last year. The measurement used the gold foil neutron activation technique. The results showed that the experimental data agreed with the simulation results very well.

5.1 Introduction to the PULSTAR UCN Source Project

Building a solid deuterium ultracold neutron source at the NCSU PULSTAR reactor is a joint project proposed by groups from the NC State Physics Department and Nuclear Engineering Department [13]. Building on our experience with the
UCNA source at LANL and collective UCN research experience, we have constructed a detailed ultracold neutron source physics model which can be coupled with other calculations to evaluate and optimize the source performance. Our UCN source model has been continuously updated as engineering has evolved.

5.2 Introduction to the PULSTAR Reactor

The NCState PULSTAR reactor is a 1 MW power reactor constructed for education and training purposes. Water is used to moderate neutrons and to cool the reactor core (see Fig. 5.2.1).

![Figure 5.2.1 NCSU PULSTAR Reactor Core](image)

Figure 5.2.1 NCSU PULSTAR Reactor Core

There are six horizontal experimental beam tubes and a thermal column arranged for access to the reactor core. The reactor core has an arrangement of 5
by 5 fuel assemblies. Each assembly contains an array of 5 by 5 fuel rods. The fuel itself is composed of either 4% or 6% enriched uranium oxide. There are two reflector walls on the outside of the core. One consists of graphite blocks, the other consists of beryllium blocks.

A MCNP model was built in the process of designing the UCN source at the PULSTAR reactor. Fig 5.2.2 depicts the MCNP configuration of the reactor core and reflectors.

![Figure 5.2.2 MCNP Model of Reactor Core](image)

For low power, low enrichment reactors, adding reflectors can increase the neutron flux in the reactor core. When neutrons escape from the reactor core, they are either absorbed by water, the reactor wall or guided outside of the reactor vessel through a guide tube. When a reflector is placed beside the core, neutrons “leaking” from the core can be reflected back into the core region. This increases the probability of interaction of the neutron with the fuel. Reflector materials usually have high scattering cross-sections and low absorption cross-sections (for example graphite, beryllium and water etc.). The larger scattering cross-section ensures a
higher probability of scattering in very small layer of the reflector near the outer boundary of the reflector. The smaller absorption cross-section decreases the neutron losses in the reflector. Also, reflectors are expected to have good moderation properties, so the high-energy, fast neutrons are moderated to thermal energies when they are reflected back to the core. Moderation ensures that the probability of resonance absorption of reflected neutrons is low, further increasing the returned flux to the core. From an engineering perspective, the reflector makes a smaller reactor core size feasible. Smaller cores conserve reactor fuel. Reflectors also ensure more uniform neutron flux density than reactors without the reflector, improving the reactivity of the core.

In the PULSTAR reactor at present, there are four neutron activation tubes outside the core (see Fig. 5.2.1) and just in front of the current noseport. The noseport is sitting on a cradle, which is made of Al and filled with graphite rods. Behind the reactor tank wall, there is a 4 ft wide by 4 ft high by 5 ft long square port in front of the concrete door, which is called the thermal column.

Figure 5.2.3 UCN source nose port
The proposed UCN source will be built inside a D2O tank and be installed inside the thermal column. The new noseport features a floodable central channel which can act as a neutron shutter. When the UCN source is not in operation the noseport can be filled with de-ionized water from the reactor vessel. When neutrons are required for the source, water can be forced out of the channel with pressurized with Helium gas.

An Al box with a 2 cm layer of lead will be installed in the gap between the noseport and the core (where the neutron activation tubes were located). The lead will serve to shield our source from core gamma-rays and act as a reflector. Details of the thermal, cold and ultracold moderators and cryostat are presented in Sec. 5.3. The UCN transport system will be a 16 cm diameter DLC-coated quartz guide system.
Before installation of our source, the thermal column was filled with many 4 inch by 4 inch cross-section, high density graphite rods. They were either 24 or 36 inches long. Within the rod assembly, there were four irradiation testing channels. Last year we used one of these channels to conduct an absolute thermal neutron flux measurement using the gold foil activation method. (Sec. 5.4)

![Thermal column](image)

Figure 5.2.5 Thermal neutron benchmark measurement

### 5.3 Monte Carlo simulation of NCSU UCN source

An MCNP simulation has been conducted with for the PULSTAR UCN source, incorporating our cryostat engineering design. This simulation includes a 4% and 6% mixed fuel arrangement, a lead box to shield the gamma heating, a new graphite filled nose port (with a He gas channel inside), and a cryostat within a 155.6 gallon D$_2$O tank. The cryostat is located near the reactor vessel liner, inside the room temperature D$_2$O moderator vessel. The cryostat itself is constructed almost entirely
of 2 mm Al tubing, with the exception of a Zr thermal break just above the SD$_2$ volume. The cold moderator is arranged in a 1.5 liter, cup-shaped volume around the SD$_2$ converter, with walls roughly 1.5 cm thick. The cold moderator can be held at temperatures down to roughly 25 K using He vapor. The SD$_2$ volume is a cylinder 17 cm in diameter and 4.5cm high with a total volume of about 1.6 liter. It is cooled by flowing liquid He, and can be frozen down to 5 K.

Figure 5.3.1 MCNP Model of the NCSU UCN source

To calculate the heat load and neutron flux, we need some factors to normalize MCNP to the absolute flux from the reactor. To normalize a criticality calculation to the steady-state reactor flux, one can assume that one fission releases 200 MeV energy, which includes the instantaneous energy from the fission process (the kinetic energy of fission products, the energy of fission neutrons, the instantaneous gamma-ray energy and the capture gamma-ray energy) and the delayed energy from fission (beta-particles from fission products, gamma-rays from fission products and neutrinos). (see Appendix B)
If the efficiency K is equal to 1, which means that there is one source neutron per fission (the remaining fission neutrons are absorbed or escape), the neutron flux of a 1 MW reactor will be $3.120 \times 10^{16} \text{ neutrons/cm}^2 \cdot \text{sec}$. Tallies are normalized to per fission neutron. To scale the tally to steady state reactor power, we assume that the fission rate is 2.418 neutrons per fission and the reactor is operated at the 1MW power level, producing a scale factor of

$$
\text{(1 Mw)} \times (3.120 \times 10^{10} \text{ fission/w-sec}) \times (2.418 \text{ neutrons/fission}) \\
= 7.544 \times 10^6 \text{ neutrons/sec}
$$

Figure 5.3.3 MCNP simulation of the cold neutron flux in the UCN source converter volume

Figure 5.3.5 depicts the MCNP model of the UCN source cryostat. We used a 17 cm diameter by 4.5 cm high, cylindrical volume filled with 5 k solid deuterium as our UCN converter. From MCNP, the cold neutron flux averaged within the SD$_2$ volume is about $0.4 \times 10^{12} \text{ CN/cc/second}$. 
1) Calculation of UCN production per cc of SD$_2$:

$$\sum \Phi_{UCN} = \frac{\rho}{A} \times N_0 \times \sum \delta_{down} \times \Phi_{CN}$$

$$= \frac{0.2 \text{ g/cm}^3}{2 \text{ g/mol}} \times 6.022 \times 10^{23} (\text{#/mol}) \times 10^{-24} (\text{cm}^2) \times \sum \delta_{down} \times \Phi_{CN}$$

$$= 7500 \text{ UCN/cc/sec} \quad (5.7)$$

Which $\rho$ = density of solid deuterium;
$\delta$ = down scattering cross section;
$N_0$ = Avogadro’s number = $6.022 \times 10^{23}$ numbers/mol.
2) Calculation of heating load: the MCNP heat tally unit is MeV/g, and the fission-heating estimate assumes that all photons are deposited locally. The source normalization and tally are consistent with the 1 MW assumed power level. So, for example, to calculate the heat load on the SD₂, we use a neutron flux of \((7.544 \times 10^{16} \text{ neutrons/sec})\) and density for the SD₂ is 0.2g/cm³. The heating result will be:

\[
H_{\text{MCNP}} \times 7.544 \times 10^{16} \times 1.602 \times 10^{-13} \times \rho \times V_{\text{volume}},
\]

(5.8)

Where \(H_{\text{MCNP}}\) is the MCNP heating tally. Sketches of the UCN guide system are depicted in Fig. 5.3.4 and Fig. 5.3.5. The UCN guide system includes quartz guides (QG), Al tubes (AG) and Zr-2 guides (ZG). The diameter of internal guides (QG) is 17cm; thickness is 2mm. The Zr-2 guides (ZG) are used for a thermal break between the SD₂ volume, cooled by LHe, and the guide walls cooled by cold He gas.

Figure 5.3.6 UCN Guides
The solid methane wall thickness is 1 cm and the bottom thickness is 9 mm. The solid methane chamber is composed of 1 mm thick Al. Outside the solid methane chamber there is a 1 mm thick Aluminum thermal shielding plate. The heat load calculations for the main source parts are listed in table 5.3.1

<table>
<thead>
<tr>
<th>Region</th>
<th>Mass(g)</th>
<th>Neutron heat load(Watt)</th>
<th>Photon heat load(Watt)</th>
<th>Total heat load(Watt)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SD2 converter</td>
<td>227</td>
<td>0.733</td>
<td>0.281</td>
<td>1.014</td>
</tr>
<tr>
<td>Solid Methane</td>
<td>614</td>
<td>1.741</td>
<td>1.232</td>
<td>2.973</td>
</tr>
<tr>
<td>Titanium tubes</td>
<td>176</td>
<td>0.003</td>
<td>0.484</td>
<td>0.487</td>
</tr>
<tr>
<td>Thermal break plate</td>
<td>884</td>
<td>0.035</td>
<td>1.221</td>
<td>1.256</td>
</tr>
<tr>
<td>Al SD2 chamber</td>
<td>601</td>
<td>0.020</td>
<td>0.916</td>
<td>0.936</td>
</tr>
<tr>
<td>Al SCH4 chamber</td>
<td>1852</td>
<td>0.066</td>
<td>2.971</td>
<td>3.037</td>
</tr>
<tr>
<td>UCN guides before the gate valve (quartz, Zr-2, Al)</td>
<td>5151</td>
<td>2.379</td>
<td>5.875</td>
<td>8.254</td>
</tr>
<tr>
<td>UCN guides outside jacket</td>
<td>3230</td>
<td>0.099</td>
<td>3.347</td>
<td>3.446</td>
</tr>
</tbody>
</table>

Table 5.3.1 Heat load simulation results

To evaluate the activation of the UCN guides and to estimate background issues, we also placed MCNP point detectors which measured the neutron flux at different positions on the edge of D₂O tank. Table 5.3.3 lists tallies without any polyethylene shielding, with “Up”, “Down” and “Middle” point detectors present (see Fig. 5.3.7).
Table 5.3.2 Background Tally I (units are neutrons/cc/sec, no polyethylene shielding)

Table 5.3.3 lists the point tallies with polyethylene shielding in place to minimize the ambient neutron flux around the guides. Even with polyethylene shielding present the background at the exit of the source guide section is still higher than we would prefer. To cut down the thermal neutron background further, improved shielding geometries around the guides must be studied.

Table 5.3.3 Background Tally Results II (units are neutrons/cc/sec, polyethylene shielding)
5.4 The Thermal Neutron Flux Benchmark Measurement and MCNP Simulation Results

5.4.1 Experimental Procedure and Calculation:

We used a sample hanger which has 29 sample positions. Each position is separated by 2 inches. During the thermal neutron measurement, we first put four gold foil samples (2 mil thickness and 1 cm² area) without Cd covers at the following locations: 2.54cm, 17.78cm, 48.26cm and 144.78cm from the internal side of the reactor walls. Samples were irradiated for about 15 minutes. After irradiation all samples were removed and stored for about 1.5 days. We used the nuclear engineering group’s shielded, calibrated Ge gamma-ray detector to measure the activation of the foil (the detector was calibrated using a 1.942 μC ¹⁵²Eu source).
The principle of gold foil activation is to count the number of $^{197}$Au atoms produced via neutron capture. The produced $^{197}$Au beta-decays and produces a prompt gamma-ray at 412.5kev. The rate of emission from the activated sample can measured using our calibrated Ge detector, and the total number of $^{197}$Au atoms can be determined. The dead time was kept smaller than 15%. A representative detector’s efficiency for the 412.5 KeV gamma-ray was established with the calibrated spacer geometries to set the distance between the foil sample and the Ge detector. For these measurements, the “spacer C” or “spacer F” geometry was used.

To measure the epithermal neutron flux, we used the same size Au foils and put them at the same positions. For this measurement, however, we placed the foils within Cd enclosures and then measured the samples for 60 minutes at a reactor power of 500 kW. The idea behind these measurements is that the Au foil can be activated by both thermal and epithermal components of the neutron flux, but we are only interested in the thermal component of the flux for our activation measurement. Because Cd has a very high thermal neutron absorption cross-section and a much smaller cross-section for epithermal neutron absorption, the Cd jackets effectively permit us to independently determine the epithermal component of the “thermal capture flux” or the total thermal neutron flux incident on Au foil that produces $^{197}$Au.

5.4.2 Irradiation Activity Calculation

To model our thermal neutron flux, we assume that neutrons in the thermal column are in thermal equilibrium with our graphite moderator, and therefore have energy and velocity distributions which conform to the Maxwell-Boltzmann distribution:

$$N(E) = \frac{2\pi}{(\kappa \pi T)^{3/2}} e^{-E/\kappa T} E^{1/2}$$

Where $N(E)$ is the neutron density and $T$ is the temperature of the moderator in Kelvins.
From $\frac{\partial N(E)}{\partial E} = 0$, the most probable energy of the thermal neutron energy distribution is $E_0 = \frac{1}{2} kT = 4.3 \times 10^{-5} \times T (eV) = 0.0125 \text{ eV}$. If $T = 293.4 \text{ K}$ and $\frac{\partial N(V)}{\partial V} = 0$, we know the most probable velocity is $V_0 = \sqrt{\frac{2E_0}{m}} = \sqrt{\frac{kT}{m}} = 2200 \text{ m/s} \ (V_0 = 1.28 \times 10^2 T)$ and corresponds to an energy of 0.0253 eV.

We note here that the real thermal neutron energy distribution may deviate from a Maxwell-Boltzmann distribution. This is because thermal neutrons are coming from the moderation of high energy neutrons. Step by step, they approach thermal equilibrium with matter. Because the distribution may not be fully “thermalized”, a relative number of high energy neutrons may be greater than predicted by a Maxwell-Boltzmann distribution. Also, it is often the case that low energy neutrons have larger absorption cross-sections than high energy neutrons, resulting in further decrease in the relative number of slow neutrons relative to faster neutrons. Both effects tend to exaggerate the high energy neutron flux relative to the M_B distribution, moving the whole thermal neutron energy spectrum to somewhat higher energies. The average thermal neutron energy and the most probable energy are higher than the average energy and most probable energy for neutrons in thermal equilibrium. This is called thermal neutron spectra “hardening”.

In general, it is traditional for capture flux measurements to consider neutron energies lower than some limiting energy “$E$”. “$E$” is called the “boundary” energy. Assuming a thermal neutron energy distribution from zero energy up to the $E$, then the thermal neutron cross section is defined as:

$$\bar{\sigma} = \frac{\int_0^E \sigma(E)N(E)VdE}{\int_0^E N(E)VdE} = \frac{\int_0^E \sigma(E)N(E)\sqrt{E}dE}{\int_0^E N(E)\sqrt{E}dE}, \quad (5.10)$$
Where now \( N(E) \) is the hardened thermal neutron M-B distribution function. If the absorption cross-section satisfies the \( 1/v \) rule, then

\[
\sigma_a(E)\sqrt{E} = \sigma_a(0.0253)\sqrt{0.0253} \tag{5.11}
\]

When the boundary energy is large enough, the part of the distribution above the boundary energy will be a small fraction of the total neutron flux, so we can extend the limit from \( E \) to infinity without significant error. Integrating equation 5.10 (after applying 5.11 to the numerator), we have

\[
\sigma_a = \frac{\sqrt{\pi}}{2} \sqrt{\frac{0.0253}{kT_n}} \sigma_a(0.0253) \tag{5.12}
\]

Where \( kT \) is 0.0253 when \( T \) equal to 293 K. Then

\[
\sigma_a = \frac{\sigma_a(0.0253)}{1.128} \sqrt{\frac{293}{T_n}} \tag{5.13}
\]

The production rate for our thermal flux of \(^{197}\text{Au}\) in our detection foils is:

\[
R = \Phi_{th}\sigma_{act}N_{\text{Au}} \tag{5.14}
\]

Where \( \Phi_{th} \) is now the thermal neutron flux \( (m^{-2}s^{-1}) \), \( \sigma_{act} \) is the differential activity cross section \( (m^2) \), and \( N_{\text{Au}} \) is atomic number of Au. During the irradiation, the net activation rate must be connected to the decay rate of the \(^{197}\text{Au}\). The population of \(^{197}\text{Au}\), \( N(t) \) is governed by the equation:

\[
\frac{dN(t)}{dt} = \Phi_{th}\sigma_{N_{\text{Au}}} - \lambda N(t) \tag{5.15}
\]
Where $\lambda$ is nuclear activity decay constant (s$^{-1}$) and $R$ is the production rate. This yields, for the population of $^{197}$Au atom,

$$N(t) = \frac{R}{\lambda}(1 - e^{-\lambda t}) ,$$

(5.16)

and after irradiation time $T$, the decay rate will be:

$$A(t) = \lambda N(T) = R(1 - e^{-\lambda t}) .$$

(5.17)

If we wait a time $\tau$ after activation before we count the sample, the activity rate will drop to:

$$A(T, \tau) = R(1 - e^{-\lambda T})e^{-\lambda \tau} ,$$

(5.18)

We must also consider the self-shielding effect, because the Au foil is not infinitely thin. The average neutron flux at the sample surface and inside of the sample will differ due to neutron absorption in the Au foil itself. The self efficiency correction factor is defined as $G_{th} = \frac{\Phi}{\Phi}$.

The activity rate is therefore

$$A(T, \tau) = \Phi \sigma N_{Au} G_{th} (1 - e^{-\lambda T})e^{-\lambda \tau} .$$

(5.19)

The number of nuclei in the Au foil is

$$N_{Au} = \frac{m \times A \times V \times \alpha}{M} ,$$

(5.20)
Where $M$ is atomic number, $m$ is sample mass, $\alpha$ is saturation, $N_{AV}$ is Avgadro constant $6.022 \times 10^{23}/\text{mol}$, and $V$ is the volume. From the Eqn. 5.18, 5.19 and 5.20, the thermal flux is

$$\Phi_{th} = \frac{2e^{2\tau}}{\sqrt{\pi} N_{Au} G_{th} \sigma (1-e^{-\lambda_T})} \sqrt{\frac{T_n}{T_0}} [A_b(\tau) - A_{cd}(\tau)], \quad (5.21)$$

Where we are subtracting the epithermal flux contribution to the activity $A_{cd}(\tau)$. A final correction must be applied for dead time, because while a gamma event in the Ge is being electronically processed and measured in the analog-to-digital converter, the electronics is effectively “dead” and can not count a second pulse which arrives during the conversion process. The results in a rate-dependent reduction in the efficiency for gamma counting, so we measure the gamma emission rate at the time $\tau$ after activation:

$$I(\tau) = \eta \cdot A(\tau), \quad (5.22)$$

Where $I(\tau)$ is gamma-ray count rate, $\eta$ is counting efficiency, which includes a correction for dead time effects. Summarizing, the production rate of $^{198}\text{Au}$ is:

$$R_{198} = \frac{m_{197} N_{AV}}{M_{197}} \langle \sigma^a \rangle \Phi_{th}, \quad (5.23)$$

So the number of Au-198 atoms after reactor irradiation is:

$$N_{198} = \frac{R_{198}}{\lambda_{198}} [1 - \exp(-\lambda_{198} T_{irr})], \quad (5.24)$$

And the activity of Au-198 after irradiation is:
The counting rate of 411 keV gamma peak, $C_{411}$, is:

$$C_{411} = A_{98} f_{411} E_{411} \exp(-\lambda_{198} T_{\text{wait}})(1 - \exp(-\lambda_{198} T_{CT})) / \lambda_{198},$$  \hspace{1cm} (5.26)$$

Where $f_{411}$ is the fraction of disintegrations that give 411 keV gammas, $E_{411}$ is the counting efficiency for 411 keV gamma which includes the solid angle fraction times detector efficiency $\eta$. We then have

$$A_{98} = C_{411} \lambda_{198} \exp(\lambda_{198} T_{\text{wait}}) / (f_{411} E_{411} (1 - \exp(-\lambda_{198} T_{CT}))),$$  \hspace{1cm} (5.27)$$

And the total neutron flux can be determined from Eqn. 5.28. The results of our thermal flux measurements are listed in table 5.4.1.

$$\Phi = \lambda_{198} M_{197} / N_{411} m_{197} \exp(\lambda_{198} T_{\text{wait}}) / [f_{411} E_{411} \langle \sigma_1 \rangle (1 - \exp(-\lambda_{198} T_{CT}))(1 - \exp(-\lambda_{198} T_{\text{Irr}}))].$$  \hspace{1cm} (5.28)$$

<table>
<thead>
<tr>
<th>Foil Mass (gram)</th>
<th>Position (cm)</th>
<th>Irradiation time (min.)</th>
<th>Waiting time (min.)</th>
<th>counting time (min.)</th>
<th>Gamma ray counts</th>
<th>Activity</th>
<th>Thermal neutron Flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.095</td>
<td>2.54</td>
<td>15</td>
<td>2667</td>
<td>5</td>
<td>278000</td>
<td>1.21E06</td>
<td>1.90E10</td>
</tr>
<tr>
<td>0.095</td>
<td>17.78</td>
<td>15</td>
<td>2675</td>
<td>5</td>
<td>150000</td>
<td>6.53E05</td>
<td>1.03E10</td>
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<td>48.26</td>
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<td>3.16E09</td>
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<td>0.095</td>
<td>144.78</td>
<td>15</td>
<td>2880</td>
<td>5</td>
<td>2.83E03</td>
<td>2.83E03</td>
<td>4.44E07</td>
</tr>
</tbody>
</table>

Table 5.4.1 Thermal Neutron Flux Measurement Result
A MCNP simulation has been conducted to benchmark the results of our thermal neutron measurements. A realistic reactor and thermal column geometry (Fig. 5.4.1) were used in the model. We simulated the thermal neutron flux in one of the testing channels. Figure 5.4.2 shows simulated thermal neutron flux results with 0.5 MW reactor power. The simulation agrees with the measurement data very well.

![Figure 5.4.1 MCNP model of the thermal neutron measurement](image1)

![Figure 5.4.2 Comparison of Measurement and simulation results](image2)
5.5 UCN Transport of the NCSU UCN Source System

An in-house UCN transport code already developed for the UCNA project was applied to the PULSTAR source. The geometry of this system is shown in Fig. 5.5.1. The SD$_2$ chamber can hold a sample of solid deuterium up to 5 cm thick (1.2 liters). We plan to coat the SD$_2$ chamber and the lowest guides of the PULSTAR source with $^{58}$Ni to minimize losses due to the boost out of the SD$_2$. For this simulation, however, we took all of the guides to be DLC-coated quartz tubes. The first section of guide is vertical, and held at low temperatures [29] by flowing He vapor coupled to the outside surface of the guides. The UCNs are then directed out through a gradual, 90 degree elbow composed of three sections to make the bend very smooth. Presumably this gradual bend will reduce the probability of UCN encountering the guide walls near normal incidence and reduce losses. Before the gate valve, there's an Al foil to separate the source and external guide vacuums.

![Figure 5.5.1 PULSTAR UCN source transport system](image)

The rest of the UCN guide system is beyond the gate valve. The inner diameter of the guide is 16 cm. For UCN transport simulations, we used a set of surface tally...
detectors to evaluate the UCN flux at different locations. The UCN lifetime inside the solid deuterium was taken to be 25 ms and the incoherent elastic scattering mean free path was taken to be 8 cm. The results are listed in table 5.5.1.

<table>
<thead>
<tr>
<th>UCN spectrum cutoff energy</th>
<th>335 neV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tally12</td>
<td>29.35%</td>
</tr>
<tr>
<td>Tally13</td>
<td>28.34%</td>
</tr>
<tr>
<td>Tally14</td>
<td>21.73%</td>
</tr>
<tr>
<td>Tally15</td>
<td>18.41%</td>
</tr>
<tr>
<td>Tally16</td>
<td>15.38%</td>
</tr>
</tbody>
</table>

Table 5.5.1 UCN transport simulation results

Contour plots of the UCN energy spectrum versus the polar angle theta are shown in Fig. 5.5.2. The polar angle is always measured relative to the guide axis (in the direction exiting the source, see Fig. 5.5.1)

![Contour plots of the UCN energy spectrum versus the polar angle theta](image)

Figure 5.5.2 UCN beam profile
We also performed transport simulations for a single energy UCN. As seen in Fig 5.5.3, UCNs are boosted as they pass through the SD\textsubscript{2} surface. The kinetic energy then drops as the UCN height increases, as expected in a gravitational field.

The UCN flux at end of the guides can be calculated from the production rate and transmission of the guide system. UCN production per cc of SD\textsubscript{2}, based on a 335 neV cutoff energy in SD\textsubscript{2} and using the incoherent approximation with the real phonon spectrum, is $\Phi_{UCN}$:

$$\Phi_{UCN} = \frac{\rho}{A} \times N_0 \times \sum \delta \times \Phi_{\text{CN}} = 7498 \text{ UCN / cc / sec} \quad (5.29)$$

assuming the UCN lifetime $\tau_{SD2}$ in the solid deuterium is 25 ms (upscattering or absorption). The limiting density for our source (the lifetime inside the solid deuterium) is $\rho_{\text{source}}$. 

![Figure 5.5.3 Single energy UCN beam profile](image_url)
\[ \rho_{\text{source}} = \Phi_{\text{UCN}} \times \tau = \Phi_{\text{UCN}} \times \tau_{SD_2} = 7498 \times 0.025 = 187 \text{ UCN/cc}. \quad (5.30) \]

If we take the UCN flux to have a cutoff energy of 335neV, there is a 15% transmission rate to get outside of reactor wall (3.6 meters away from UCN source). Then the UCN density in the guide system outside the reactor wall is:

\[ \rho = \rho_{\text{source}} \times \eta = 187 \times 0.15 = 28 \text{ UCN/cc}, \quad (5.31) \]

assuming losses in the guide are small. If we use a higher UCN cutoff energy, the UCN density inside of SD$_2$ will be higher due to a larger down-scattering cross section. The transmission, however, will be lower because the higher energy neutrons will not be stored in the guide system if their energy is greater than the Fermi potential for the guide wall.
Chapter 6

Monte-Carlo Analysis of the ILL Ultracold Neutron Depolarization Measurement

Measurements and analysis of DLC-coated quartz guide tubes is an essential component of the UCNA experiment. High transmissions for UCN through our guide system are necessary to ensure adequate decay rates in our decay “bottle”. Also, to ensure our systematic errors are well below our targeted 0.2%, we must maintain 99.9% polarization of UCN in our decay volume for residency times of roughly 5 s. In 2001 and 2002, measurements of depolarization and transmissions for our DLC guides were performed at ILL. The UCN Monte Carlo transport code discussed in Chapter 3 was first developed to analyze the results of these measurements. After carefully comparing the measured data with the results of our simulation, we extracted a depolarization rate for DLC-coated quartz guide of about $1.2 \times 10^{-6}$ per bounce. The UCN guide transmissions are consistent with measured values for a range of specularities from 0.9905 to 0.9953 (depending on the specularity model used).

6.1 Mechanical Turbine UCN Source at ILL

The ILL serves a primarily materials and condensed-matter research community through a variety of neutron sources coupled to a 60 MW research reactor. Thermal neutrons at a temperature of roughly 300 K, (energies of about 25
meV) are produced directly by the heavy water moderator inside of the reactor tank. The neutron flux at the reactor core is about $10^{15}/\text{cm}^2/\text{second}$. There are two liquid deuterium cold neutron sources inside the reactor. The cold neutron moderators shift the neutron energy distribution towards lower energies, increasing the number of long wavelength neutrons available for materials and condensed matter research. The flux is about $10^{10}/\text{cm}^2/\text{s}$ at the face of the cold source [67].

Ultracold neutrons with energies below $3.3\times10^{-7}$ eV are only a very small fraction of the total neutron flux in a typical liquid deuterium cold source. In order to increase the flux of ultracold neutrons, a mechanical turbine is used to slow down VCN and make lower energy VCN and UCN. Figure 6.1.1 shows a cross-section view of the ILL reactor and mechanical turbine UCN source [72].

Figure 6.1.1 ILL UCN Source
Neutrons moderated by the cold neutron source are extracted vertically through a nose-shaped, 1mm thick aluminum vacuum tube. They then enter a vertical neutron guide system which includes two sections: the lower section is composed of multiple sections of 7 cm diameter, nickel-coated guide (a total of 5 m in length), and the upper section is composed of 7 cm by 7 cm curved guides (a total of 13 m long). These curved guides effectively reduce gamma ray and high energy neutron background in the guide hall, situated on the top floor of the reactor facility. The vertical rise permits one to extract neutrons at energies considerably higher than UCN (the neutrons lose 100 neV/m over 17 m increasing vertical height) and where the neutron flux is much higher than at UCN energies. To further increase the VCN density, neutrons exiting the guide are directed into a mechanical turbine developed by A Steyerl. The principle can be interpreted using energy conservation. Neutrons exit the guide system with velocity \( u \), then strike a turbine blade with velocity \( v \) moving in the same direction as the incident neutrons. The reflection from the blade surface is elastic and results in \( 2v-u \) in the neutron velocity moving in the opposite direction (in the frame of blade). Those VCNs at velocities of roughly 50 m/s are slowed to UCNs (about 5 m/s) by multiple reflections from the nickel-coated turbine blades. The result is a larger UCN phase speed density at the turbine exits for UCN experiments. The maximum UCN bottleable density at the exit is about 40 UCN/cm\(^3\)[67].

### 6.2 UCN Transport Measurement at ILL

The geometry of our transport measurement at ILL is shown in Fig. 6.2.1. UCN exiting the mechanical turbine enter a gravitational spectrometer consisting of a Be-coated bottle with a movable absorber at the top. This spectrometer can be used to measure the ultracold neutron energy spectrum directed into the spectrometer or to
prepare a spectrum of UCN with specific cut-off energy for subsequent experiments. At one exit of this spectrometer we connected a 1m section of $^{58}\text{Ni}$ coated S.S. guide coupled to a shutter, and then two sections of DLC-coated quartz guides. We then coupled a $^3\text{He}$ UCN detector with a 0.6 cm diameter polyethylene aperture at end of the DLC guides (see Figure 6.2.1).

The transmission was calculated by taking the ratio of the measured flux with guide C in place to the flux measured with guide C removed. The baseline flux with guide C removed changed very little. The cut-off energy was caused to vary in these measurements by varying the absorber height. The height was measured from the center of our extraction guide, so the potential energy was just $m \times g \times h = 0.1 \text{ neV/mm}$. Based on the measured data, the energy-averaged transmission of our best DLC-coated guide sections was about $0.945 \pm 0.005$. 
Figure 6.2.2 Measured UCN transmission for our best DLC-coated guide as a function of absorber height in the gravitational spectrometer

6.2.1 UCN Transport Simulation

To simulate the UCN transport, we used a simplified geometry with a $^{58}\text{Ni}$-coated, 1m long, 3.91 cm radius guide A; a 1.14m long 3.2cm radius DLC-coated guide B; and a standard, 0.946m long, 3.2cm radius diamond-like-carbon coated guide C in front of the detector (Guide B included roughly 20 cm of DLC guide inside our neutron shutter). We tested UCN incident on the Al entrance foil to the detector to see if the UCNs reflected from the foil surface using the treatment discussed in Sec. 3.2 (for a single layer Al foil). Those ultracold neutrons passing through the foil are modeled as being detected with 50% absolute detection efficiency. (This is arbitrary, because we did not implement energy dependence to the subsequent detection in the $^3\text{He}$ detector once the UCN passed the foil.)
The initial UCN spectrum was measured by Vasiliev et al. using the UCN spectrometer. UCN counts at different height of the absorber give the UCN density distribution as a function of energy. Fig. 6.2.4 depicts the measured distributions for the spectrometer and the spectrometer with various Al exit foils, as well as the equation that we use to sample UCN energy in our transport code.

![Differential spectrum](image)

**Figure 6.2.3 Measured UCN spectrum at ILL**

We then modeled our UCN transport measurements for several different assumptions about the guide specularities. The simulated value of the transmission was taken from the ratio of the simulated flux with all guides in place over the simulated flux without guide C.

Three different cases were simulated: 1) both guide B and guide C having the same specularity; 2) guide B’s specularity fixed at 0.98 and guide C’s specularity varying; 3) guide B’s specularity fixed at 0.995 and guide C’s specularity varying. For these tests, the probability of non-specular scattering was taken as a simple constant, independent of energy and incident angle, and non-specularly scattered UCN have an isotropic angular distribution (in the half-space above the guide
surface). Using the widest range of values accommodating an increase of $\chi^2$ by 1 of all data sets gave us an overall range of specularities consistent with our measured value of the transmission ($0.945 \pm 0.005$) of .9905 to .9953. This result agrees very well with our assumptions in the analysis. We also conducted the same kind of simulation using a Be-energy cut-off in the input energy spectrum. A comparison with the experimentally determined transmission rate of 0.945, indicated a small specularity increase to 0.9915~0.9965 within our 68% confidence level limits.

![Figure 6.2.4 UCN spectrum models used in the simulation](image)

Discussion of Non-specular scattering:

Although UCN scattering from the surface is almost entirely specular in nature, there is always a small amount of non-specular scattering (about 1%) present. The rate of non-specular scattering is determined by the surface properties (for example, the correlation length or short-distance fluctuation) and the incident neutron energy. Because our guide surface is very smooth and the measured guide sections are short, it is challenging to extract any details concerning the energy and angular dependence of non-specular scattering present in these guides.
Figure 6.2.5 Monte-Carlo transmission simulation with a UCN energy distribution having a Cu cut-off

Figure 6.2.6 Monte-Carlo transmission simulation with a UCN energy distribution having a Be cut-off
6.3 UCN Depolarization Measurements at ILL

UCN depolarization result from wall collisions, from inhomogeneities in the magnetic field, and from wall collisions in the presence of magnetic field gradients. Here, because estimates indicate the magnetic field-induced depolarization mechanisms are negligible, we focus on depolarization resulting from collisions with the wall only. Aspects of these measurements have been presented in previous dissertations by M. Makela [36], C. Y. Liu [32] and from a small set of previous measurements [10, 51, 52].

6.3.1 The measurement setup

In this measurement, the input spectrum was either conditioned by filling and storing UCN in the spectrometer before admitting them to the depolarization test guides (for the AFP “off” case), or by continuously flowing UCN through the spectrometer and into the test guides, with roughly the same resulting spectrum (for the AFP “on” case). When the spectrum was conditioned, the spectrometer was filled and then UCN stored for 50 s. The experimental volume was then typically “loaded” for 120 s, allowing the UCN to flow into our PLD guides through the polarizing magnet (only the spin state polarized antiparallel to the field passed through the magnet). The switcher was then activated, and the UCN valve to the spectrometer closed, stopping the loading process and allowing UCN which could still pass through the magnet (if they were still polarized antiparallel to the field) to drain to detector 2 (see Fig. 6.3.1). The switcher’s state change took less than 0.5 s. An important detail for the UCN transport model was the presence of a stainless steel “T” at the exit of the switcher. This guide element coupled the $^{58}$Ni exit guide of the switcher to a S.S. pumping port and to our DLC guide. Although this component was electropolished, the specularity of its surface was not known.
Figure 6.3.1 Geometry of the ILL depolarization measurement

The magnet serves, for the depolarization measurements, as both a polarizer and an analyzer. UCN were polarized by passing the UCN guide through the high magnetic field region of a warm bore, superconducting magnet with a roughly uniform 5T field over a 10 cm region along the field axis of the magnet. The UCN would experience a potential of \( V = \mu \cdot B \) where \( \mu = -1.9 \mu_N \), and \(|\mu_N| = 30 \text{ neV/T} \).

Hence spins anti-parallel to the field ("right spin" UCN) were accelerated into the high field region and passed through the polarizing field effectively unhindered. Spins parallel to the field experience a potential barrier and are repelled. As long as the kinetic energy of the UCN incident on the field is less than 300 neV, UCN entering the bottle should be fully polarized. As Fig. 6.2.3 indicates, the input spectrum had a maximum UCN energy well below 300 neV. With the magnet field energized, only “right” spin neutrons enter the DLC-coated guides beyond the high field region (the bottle volume). UCN in this region can depolarize via wall collisions with the DLC guide material, in which case they were trapped between the magnetic field region and the back plate depicted in Fig. 6.3.1 (the “bottle”). Neutrons which did not depolarize were free to eventually return to the spectrometer. The UCN
density in the bottle volume was monitored through a 0.8 cm diameter hole in the back plate of the bottle volume. Outside of the DLC-coated guide, an RF spin flipper was situated near the center of the bottle.

6.3.2 AFP “Off” Case

For these measurements, the AFP spin-flipper was off during the loading process. Loading ended after 120 s, and switcher state was changed to direct UCN to detector 2. UCN which depolarized while they were resident in the bottle region were trapped by the polarizing magnet field and accumulated in the bottle. “Right spin” neutrons were free to leave the trap, and drained out with a characteristic drain time of about 8 s, making the large signal observed in detector 2 immediately after the switcher changed the state at 170 s (see Fig. 6.3.3).

![Figure 6.3.2 the First UCN Depolarization Measurement Time Scale](image)

**Figure 6.3.2 the First UCN Depolarization Measurement Time Scale**

![Figure 6.3.3 Detector signals for the AFP “off” case](image)

**Figure 6.3.3 Detector signals for the AFP “off” case**
In fact, we found that the “right spin” draining process was well-fit to a two component exponential dominated by the longer decay time of $8.0 \pm 0.4 \text{s}$ (see Fig. 6.3.4).

At 140 s after the switcher changed state, the RF spin flipper was energized with fields of a few G in strength, adequate to ensure very high spin-flipping probability. Thus wrong spin neutrons occupying roughly half the bottle volume did drain out of the bottle after passing through the flipper. Because the spin flip probability was very close to 100%, wrong spins which traversed the flipper twice returned to the wrong spin state, and remained trapped. When the RF flipper was finally turned off after 40 s, those UCNs currently in a wrong spin state could also escape, producing a second peak in signal (see, for example, Fig. 6.3.5, where the AFP emptying signal is large and the double peak is obvious).
6.3.3 AFP “On” Case

For this measurement after 80 seconds of loading, the AFP spin flipper was turned on. Having the spin-flipper on ensured the accumulation of a large population of wrong spin UCN in the bottle. After 120 s, the switcher state was changed to detector 2 and the spin-flipper was tuned off. The “right” spin UCN drained to detector 2, making the first peak of detector 2 signals.

![Figure 6.3.5 The AFP “on” depolarization measurement time scale](image)

![Figure 6.3.6 ILL UCN AFP on depolarization rate measurement result](image)

In this case, the bottle was now loaded with a large population of wrong spin neutrons which were trapped in the bottle, behind the polarizing field. The depolarization rate could be determined from the limiting rate at which wrong spin
neutrons depolarized and then left the trap. Hence, the experimental procedure was to determine the leak rate out of our bottle as a function of time for a series of storage times. These data also permitted us to directly determine the storage time for the wrong spin UCN in our bottle. After storage, the wrong spin UCNs were unloaded from the trap in the same manner as the AFP off case by turning on the AFP spin flipper for 40 s. The double-peaked structure of the unloaded UCN is pronounced for these data.

Because of the large population in the bottle, it was possible to determine the UCN storage time, \( \tau \), in the bottle from detector 3 signals, then fit to a two component exponential. We determined a lifetime of about 8 s and 57 s with roughly equal weight, consistent with our expectations for this system. Also note that for these measurements, UCNs were not stored in the spectrometer, but flux from the turbine source just flowed through the spectrometer. The drain time fits indicate that the procedure did not produce sizable shifts in the spectrum of UCN used in our depolarization measurement.

![Figure 6.3.7 UCN lifetime for wrong spin neutrons trapped in the bottle volume](image)

Figure 6.3.7 UCN lifetime for wrong spin neutrons trapped in the bottle volume
6.4 UCN Depolarization Analysis

6.4.1 Depolarization Rate Calculation

One of the primary goals of our analysis is to extract the depolarization probability per bounce for UCN. To determine this quantity, we need to extract the probability a given right spin neutron depolarizing in the DLC region and the number of times it bounces off of the wall.

The collision frequency is referred to as $\nu = \frac{\langle V_{\perp} \rangle}{d}$, where $V_{\perp}$ is an effective average velocity perpendicular to the DLC guide storage region wall and $d$ is diameter of the storage region (here is diameter of DLC coated guide). We can estimate this rate by assuming right spin UCN entering the trap have an effective pitch angle of about $45^\circ$ and the input UCN spectrum is associated with a Be cut-off energy. To determine the average velocity, we can histogram the energy of the UCN while they are in the bottle region and calculate the average velocity:

$$V(E)_{\text{average}} = \frac{\sum N_{\text{UCN}} \times V(E_{\text{UCN}})}{\sum N_{\text{UCN}}}$$  \hspace{1cm} (6.1)

The ultracold neutrons' average velocity is about 4.2 meters per second for the Cu spectrum. For the Be spectrum, we have an average UCN velocity of about 4.89 meters per second. The frequency $\nu$ for the Cu spectrum is 46 bounces per second, and for the Be spectrum is 54 bounces per second.

If we use a $\nu^2 \, dv$ velocity distribution, then the average velocity is

$$\nu = \frac{\int_0^{v_m} v^3 \, dv}{\int_0^{v_m} v^2 \, dv} = 0.75 \times \nu_m.$$ \hspace{1cm} (6.2)
For a Be cut-off energy of 252 neV, the average velocity is about 5.2 meters per second. The average bounce rate is about 57 bounces per second. For a Cu cut-off energy of 152 neV, the average velocity is about 4.1 meters per second, the average bounce rate is about 45 bounces per second.

If we consider the UCN as behaving like a gas, we can use gas kinetic theory to calculate the collision frequency:

\[ \nu = \frac{v_{\text{average}} \times S}{4V_{\text{volume}}} \]  

where S is the guide surface and V is the guide volume. Using this approach, the collision frequency \( \nu \) for the Cu spectrum is 43 /s, the collision frequency \( \nu \) for the Be spectrum is 49 /s. Ultimately, our extracted value for the depolarization probability is inversely proportional to \( \nu \), making it a critical parameter in the extraction of the depolarization per bounce. In the course of the analysis of our experimental data, we determined from the best-fit to simulations a collision frequency 45 /s (discussed in Sec. 6.4.2).

In the experiment, we could not directly determine the collision frequency. To extract a depolarization probability (per incident neutron), we assumed the depolarization probability was proportional to the ratio of the peak of detector 2 (the right spin neutrons in the bottle) to the second and third peaks in detector 2 (the wrong spin UCN accumulated in the trap) with both signals corrected for the storage lifetime in the bottle. To analyze the experiment, we can write the depolarization probability per bounce (uncorrected for the storage time) as

\[ \alpha_{\text{dep}} \propto \frac{A_2^e - A_b^e}{A_1^e - A_b^e} , \]  

(6.4)
where $\alpha_{\text{dep}}^s$ is DLC depolarization probability, $A_2^s$ is the second peak in detector 2, $A_1^s$ is the first peak in detector 2, and $A_0^s$ is the detector background. The simulated depolarization rate can be expressed as:

$$\alpha_{\text{dep}}^s \propto \frac{A_2^s}{A_1^s}, \quad (6.5)$$

where $\alpha_{\text{dep}}^s$ is DLC depolarization probability, $A_2^s$ is the second peak in detector 2 in our simulation and $A_1^s$ is the first peak in detector 2 in our simulation.

![Figure 6.4.1 Detector Two Background Fitting Curve](image)

**Figure 6.4.1 Detector Two Background Fitting Curve**

Our strategy is to scale our simulated ratio (Eqn. 6.4) to agree with our measured ratio (Eqn. 6.3). This permits us to incorporate the physics of the storage and spectrum into our simulation and dependence on detector efficiencies. In this thesis, we only utilize the AFP off case to extract the depolarization rate, because of the sensitivity of the AFP on case to backgrounds and marginally trapped UCN in the bottle. We extracted from the experimental data the integral number in each peak by
fitting the signals for backgrounds and thus subtracting the integrated background from the peak integrals.

\[
\frac{\alpha_{\text{dep}}}{\alpha_{\text{dep}}^{(2)}} = \frac{A_2^e - A_2^b}{A_1^e - A_1^b} \left( \frac{A_2^e}{A_1^e} \right) = \left( \frac{A_2^e - A_2^b}{A_1^e - A_1^b} \right) A_2^e
\]

(6.6)

We note here that the depolarization rate which we extract from the ratio of the second to the first peak in detector 2 is only an upper bound on the depolarization rate due to collisions with DLC surfaces. Other sources of depolarization, such as the presence of magnetic field gradients, our stainless steel coupler and surface contamination with hydrogen-rich components, may contribute to the depolarization rate at the same level, making our measurement effectively a system depolarization rate. In order to make our treatment as robust as possible, in our Monte Carlo treatment we must address the uncertainties in our geometry which affect transport, such as the specularity of our stainless steel coupler and the \(^{58}\text{Ni}\) coated guides and the loss per bounce for depolarized UCN stored in our bottle. We also took some care to assess the effect of the loading time on the bottled UCN spectra, to ensure we accurately modeled the depolarized UCN trapped in our bottle.

6.4.2 Simulation of ILL UCN Depolarization Measurement

Before ultracold neutrons entered the experimental system, they were stored inside the UCN reservoir coated with Be. The spectrum data depicted in Fig. 6.2.3 were taken during the 2002 runs at ILL, with a fresh Be coating cut-off about 252 neV. Because some damage (coating puckering) was observed of the coating in the spectrometer during the depolarization runs in 2001, we also investigated simulations in which the spectrometer chamber substrate (Cu) was exposed. Cu spectrum has cut-off energy of 153 neV. Also the height of reservoir exit reduces cutoff potential from the measured spectrum by about 25neV.

The UCN transport system includes a set of DLC-coated quartz guides. For the DLC guides, we had independent data (Sec. 6.2) which we have used to determine
the guide specularity and loss rate. We have also characterized the $^{58}\text{Ni}$ guides (or similar guides) we used in the measurement on previous occasions. We were also interested in the effect of specularity variations in the $^{58}\text{Ni}$ coated stainless steel guides, which connected detector two and the DLC-coated guides. We investigated two values for the specularity of these guides, based on our previous experience: 97.5% and 95% (constant non-specular scattering probability and isotropic scattered UCN distribution). For each choice, we varied the coupler specularity and calculated the reduced $\chi^2$ to our simulated bottle draining data. Our best fit (reducing $\chi^2 = 0.7$) used a Be cut-off spectrum, $^{58}\text{Ni}$ specularity of 0.975, and S.S. coupler specularity of 0.6. A great deal of uncertainty exists concerning the specularity of the stainless steel coupler between the switcher and our DLC guides. Although it was electropolished, the specularity is essentially unconstrained so we left it as a free parameter in our simulations, and used experimental data to determine best fit values (we evaluated $\chi^2$ for fits to the detector 2 drain data associated with peak $A_1$).

Figure 6.4.2 Chi-square for comparison between simulated right spin UCN draining from the bottle to detector 2 and experimental data.
Figure 6.4.3 Comparison between simulated right spin UCN draining from the bottle to detector 2 and experimental data.

We also simulated the UCN losses in the bottle volume to extract a characteristic storage time for wrong spin UCN. As mentioned previously, according to the detector 3 data, the decay time is about 57 seconds. Because detector 3 has very few UCN counts in a typical simulation, we used a virtual detector to simulate a response proportional to the true detector 3 signal. This virtual detector (detector 4) is a surface tally detector at the back plate of storage region used in place of the small aperture in the back plate to detector 3. Detector 4 has same function as detector 3, which is to monitor the UCN density in the storage region, but with more tallied UCN. Note: detector 4 only tallied the number of UCN hitting the end plate of the bottle volume, and did not kill UCN during the simulation. This was an efficient way to short simulations to get a robust result for the signal anticipated in detector 3. These simulations indicated an emptying time for detector 2 of 8.9 s, consistent with experiment.
The UCN bounce frequency inside the storage volume also has been simulated. The time-averaged bounces per second is 45 bounces per second for a Cu spectrum and 55 bounces per second for a Be spectrum (with the Be spectrum providing the better fit to the data). Note, a strong softening of the bottled spectrum was observed as the loading time was increased. Reasonable $\chi^2$ was not obtained until loading times approaching 120 s (the true loading times) were used.
Finally, using Eqn. 6.5, we extracted a UCN depolarization rate about $1.2 \times 10^{-6}$ per bounce. We note that the average level of the backgrounds for long emptying times was much larger than can be explained by residual UCN transport issues, and was probably due to ambient backgrounds in the guide hall.

Figure 6.4.6 Comparison of measured and simulated UCN Depolarization Results (note: the depolarization rate is obtained by scaling the simulated depolarization signal to agree with the experimental signal).

Discussion:

We also used some non-specular scattering models which did not use a constant scattering probability and isotropic scattering (the diffusion type of non-specular scattering model mentioned in Chapter 3). For example, we used a non-specular scattering model where the probability of scattering was proportional to $\cos(\theta)$, where $\theta$ is the angle of incidence and the scattered neutron had a $\cos^2(\theta)$ distribution. By comparing the two sets of simulations to the detector 2 drain data,
the reduced $\chi^2$ was determined and is shown in figure 7.1.1. For large values of the specularity (corresponding to very small probabilities of non-specular scattering), the more detailed model provides $\chi^2$’s in agreement with the best result of a diffusion-type non-specular scattering model.

Figure 6.4.7 Non-specular scattering model results
Chapter 7

Summary and Discussion

For the UCNA source project, both enlarging the W target size and putting a high density poly insert into the UCN source will increase CN and UCN production. A W target upgrade would involve significant effort both in hardware modifications to the target system and in radioisotope inventory calculations. These modifications, however, should result in UCN production can be increases from a factor of two to five, depending upon the details of the upgrade plan. It also appears that the DLC coating for the guides in our horizontal guide system are probably too thin. At the time of this writing, this is not been directly confirmed, but new guides have been produced with significantly better transmission performance for UCN at energies between 80 neV and 180 neV. We have replaced the DLC guides with polished S.S. guides for the horizontal system as well, and have observed at least a factor of 1.7 increase in UCN flux. If remains to be seen what the full recovery factor will be.

For NCSU’s UCN source project, the MCNP model of the NCSU UCN source gives a very good prediction of thermal neutron flux. UCN production is about 7500~12000 UCN/cc/s based on the existing engineering design. The range of values comes from different aspects of UCN down-scattering calculation. The UCN transport system is a work in progress.

For the ILL depolarization measurement, we finally extracted the DLC-coated quartz guide UCN depolarization rate by comparing the experiment results with simulation data. The depolarization rate was about $1.2 \times 10^{-6}$ per bounce.
Appendix A: UCNA Experiment

A neutron decays via the weak interaction into an electron, a proton, and an electron anti-neutrino. The decay rate depends on the polarization of the neutron and the momenta of the outgoing electron and anti-neutrino.

In the standard model, we have:

\[
d\Gamma \propto p_e E_e \left( E_{\text{max}} - E_e \right)^2 \left[ 1 + a \frac{\vec{P}_e \cdot \vec{P}_\nu}{E_e E_\nu} + \langle \vec{\sigma} \rangle \cdot \left( A \frac{\vec{P}_e}{E_e} + B \frac{\vec{P}_\nu}{E_\nu} \right) \right] dE_e d\Omega_e d\Omega_\nu
\]

The total rate (the lifetime) and all of the above correlation parameters are determined by the vector (\(G_V\)) and axial-vector (\(G_A\)) couplings, for example:

\[
A = -2 \frac{G_A^2 - |G_A G_\nu|}{G_\nu^2 + 3G_A^2}, \quad ft_n = \frac{K}{G_\nu^2 + 3G_A^2}
\]

The “beta-asymmetry” parameter \(A\) is one of the most sensitive of the correlation parameters to \(G_A\). This parameter represents correlation between the electron momentum and the neutron polarization. By the conserved vector current theorem, the neutron coupling constant \(G_\nu\) is related to the fundamental quark coupling. \(G_\nu\) is therefore related to the element \(V_{ud}\) of the Cabibbo-Kobayashi-Maskawa (CKM) matrix by the relationship, \(G_\nu = G_F V_{ud}\), with

\[
\begin{aligned}
&\begin{pmatrix}
d_w \\
s_w \\
b_w
\end{pmatrix} = \\
&\begin{pmatrix}
V_{ud} & V_{us} & V_{ub} \\
V_{cd} & V_{cs} & V_{cb} \\
V_{td} & V_{ts} & V_{tb}
\end{pmatrix}
\begin{pmatrix}
d \\
s \\
b
\end{pmatrix}
\end{aligned}
\]

In the standard model of particle physics, the CKM matrix must be unitary, so, theoretically:

\[
|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 1
\]
With precise measurements of $V_{ud}$ and $V_{us}$, we can test this.

![Graph showing $V_{ud}$ vs. $|G_A/G_V|$](image)

Figure A.1. Decay constant and CKM unitarity

There is currently a lack of self-consistency between neutron experiments determining the $A$ coefficient. The most precise measurement of $A$ tends to give a value for $V_{ud}$ in disagreement with results from superallowed nuclear decay. UCNA aims to settle these discrepancies with a 0.2% measurement of $A$. [1, 3, 14, 30, 37, 46, 49, 71]

![Side View of Decay trap of UCNA Experiment](image)

Figure A.2 Side View of Decay trap of UCNA Experiment
Appendix B: MCNP and MCNPX

1. MCNP Introduction:

MCNP is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. The code treats an arbitrary three-dimensional configuration of materials in geometric cells bounded by first and second degree surfaces.

Point-wise cross section data are used. For neutrons, all cross sections are tabulated in evaluation sets such as ENDF/B-VI. Thermal neutrons are described by both free gas and \( S(\alpha, \beta) \) models. For photons, the code takes account of incoherent and coherent scattering, the possibility of fluorescence after photoelectric absorption, absorption in pair production with local emission of annihilation radiation, and bremsstrahlung. A continuous slowing down model is used for electron transport that includes positrons, x-rays, and bremsstrahlung but does not include external or self-induced fields.

Important standard features that make MCNP very versatile and easy to use include a powerful general source, a criticality source, and surface source; both geometry and output tally plotters; a rich collection of variance reduction techniques; a flexible tally structure; and an extensive collection of cross section data.

2. MCNP Tally Principles:

In MCNP, the neutron flux is tallied using average track length estimation, (“F4 tally”)

\[
\overline{\phi_v} = \frac{1}{V} \int dE \int dt \int dV \int d\Omega \psi(r, \hat{\Omega}, E, t)
\]  

(B.1)
Where $\phi_\Omega$ is the average flux in a cell, $V$ is the volume, $i$ is particle position vector, $\hat{\Omega}$ is the direction vector, $E$ is the energy, and $t$ is time. $\psi$ is the angular flux:

$$\psi(r, \Omega, E, t) = vn(r, \hat{\Omega}, E, t),$$  \hspace{1cm} (B.2)

Where $n$ is the particle density (particles/cm$^3$/MeV/steradian) and $v$ is velocity in cm/10$^{-8}$ sec. The units of $\psi$ are particles/cm$^2$/10$^{-8}$sec/MeV/steradian. The integration is over time, energy and averaged over the volume. For tallied neutrons, the MCNP code actually integrates the track length density in a tally volume.

$$\frac{1}{V} \int dE \int dV \int d\Omega \int dt [vn(r, \hat{\Omega}, E, t)] = \frac{1}{V} \int dE \int dV \int ds [N(r, E, t)],$$  \hspace{1cm} (B.3)

Where $ds$ is the differential unit of track length and $ds = vdt$. The average flux can be estimated by summing track lengths for all particles in a cell. The results are very reliable since there are many tracks in a cell giving contributions.

To calculate the heat load, we use the “F6” tally. F6 heating and energy deposition tallies are track length flux tallies modified to tally a reaction rate convolved with an energy-dependent heating function. The heating tallies are flux tallies multiplied by the energy-dependent multiplier. The units of heating tally are MeV per gram. The average energy deposited for all reactions at the incident particle energy is used in the tally.

For neutrons, the heating multiplier is described as:

$$H(E) = E - \sum_i P_i(E)[\bar{E}_{i,\text{out}}(E) - Q_i + \bar{E}_{i,\gamma}(E)],$$  \hspace{1cm} (B.4)
Where \( P_i = \frac{\sigma_i(E)}{\sigma_T(E)} \) is the probability of reaction i at neutron incident energy;

\( \bar{E}_{i,\text{out}}(E) \) is the average exiting neutron energy for reaction i at neutron incident energy E; \( Q_i \) is the Q-value of reaction i; \( \bar{E}_{i,\gamma}(E) \) is the average exiting gamma energy for reaction i at neutron incident energy E.

For gammas, the heating multiplier \( H(E) \) is

\[
H(E) = E - \sum_{i=1}^{3} P_i(E)[\bar{E}_{i,\text{out}}(E)]
\]  

(\text{B.5})

\( i = 1 \) is incoherent (Compton) scattering with form factors; \( i = 2 \) is pair production, \( \bar{E}_{i,\text{out}}(E) = 2m_e c^2 = 1.022 \text{MeV} \) (is the rest-mass energy of an electron); \( i = 3 \) is photoelectric absorption.
Appendix C: Cross Section for our MCNP Simulation

We used thermal $S(\alpha, \beta)$ type cross sections for our MCNP simulations. These cross sections were calculated using NJOY [25].

Figure C.1. Solid deuterium (5 K) total cross section

Figure C.2. Polyethylene (77 K) total cross section
Figure C.3. Polyethylene (4 K) total cross section
Appendix D: Para Deuterium Fraction

1. Analysis:

Deuterium gas samples are taken from D$_2$ vapor evaporated from the source and brought to have a Raman scan. A typical Raman spectrum was similar to the one below (Raman scan results in June 2005 without an HD peak).

![Figure D.1 Raman Spectrometer](image)

![Figure D.2 Raman Spectrum Results of Deuterium Gas](image)
The para-fraction (concentration of para-D\textsubscript{2} divided by concentration of ortho-D\textsubscript{2}) is given by

\[ f = \frac{N_{p_2}}{N_{p_1}} \eta = \frac{x}{1 - x} \eta \]

Where epsilon is a constant related to the details of the Raman cross-sections and the spectrometer efficiency and \( r \) is the ratio of the ortho and para populations. The measured fraction, \( f \) is related to the ratio in the populations, \( r \) by

\[ \frac{r}{f} = \frac{0.5}{f_0} \]

With the true ratio, \( r \), we can define the Para fraction, \( x \):

\[ x = \frac{r}{1 + r} \]

The uncertainty in \( x \) is:

\[ \delta x = \frac{\delta r}{(1 + r)^2} \]

And the uncertainty in \( f \) is:

\[ \delta f = f \left( \frac{N_{p_1}}{N_{p_2}} \right)^2 + \left( \frac{\delta N_{p_2}}{N_{p_2}} \right)^2 \]
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