A Very Cold Neutron Source, VCNS

Workshop on Applications of a Very Cold Neutron Source
Argonne National Laboratory
22-24 August 2005
We have convened this Workshop and we are all here to determine whether there is enough in the VCNS technical concept and enough prospect for scientific applications to justify further inquiry into VCNS.
VCNS: Motivation

The practical motivation for this study is to establish the prospects for a neutron source providing intense pulsed beams with spectra as cold as is realistic.

The philosophical motivation is to continue Argonne’s long tradition in the development and use of neutron sources and techniques.

The scientific motivation is to serve applications in nanoscience, biology, and technology.

The vision is that of a facility at Argonne National Laboratory providing unique neutron scattering capabilities to the international community toward the end of the next decade.
VCNS: Preliminary Considerations

• “As cold as is realistic” means 2-4 K, that is, a moderator at the temperature of liquid helium. Multi-kW L-He refrigerators exist at many installations, for example in the L-He-cooled cold sections of high-power particle accelerators.

• Preliminary studies lead to bismuth as target material and as fast-neutron shield, and to a 2-to-4 K pebble-bed of D$_2$O ice (but maybe solid D$_2$, Be, or CD$_4$) moderator cooled by flowing L-He.

• The response time of a 2-K D$_2$O moderator, about 4 msec, indicates a “long-pulse” operating mode. Long-wavelength (~ 20 Å) neutrons require long interpulse intervals, therefore a low pulsing frequency.

• We assume a 300 kW proton beam, 4-msec pulse width and 1-Hz pulsing frequency, indicating a linac accelerator driver.
For Reference

The energy of 2.2 K neutrons is 190 $\mu$eV;
The wavelength is 20.8 Å;
The speed is 190. m/sec.
VCNS: Safe Observations

• Production of large quantities of mm-scale, solid pellets (CO$_2$, CH$_4$, NH$_3$, D$_2$, … ) is an established technology (CAF, Inc, Oak Ridge). The same technology should be applicable to D$_2$O, which would produce low-density amorphous (LDA) ice.

• Target technology presents no challenges and has already been demonstrated at comparable scale. (200 kW at TTNF at TRIUMF, Vancouver, ~ 1990)

• A prolific source of Very Cold Neutrons ( wavelengths ~ 20 Å, energies ~ 100 µeV) will serve applications in studies of large structures and slow motions.

• Ongoing activities in developing Ultra Cold Neutron (UCN) facilities are relevant and will be helpful.
VCNS: Challenges

- Neutronic simulations require scattering kernels that don’t exist for the temperatures of interest—developing these kernels requires considerable effort.

- Data on low-temperature thermal conductivities and specific heats of candidate moderator materials are sparse, yet essential to evaluating static and dynamic effects of moderator heating.

- Heat transfer calculations for L-He cooling is a special field, e.g. in superconducting accelerator components.
VCNS: Challenges, more

- There is little or no experience with neutron scattering instruments suitable for the expected scientific applications and for use of very cold neutrons in the long-pulse mode.

- Instruments are likely to rest heavily on neutron optical devices, all of which work better at long than at short wavelengths. Gravity will play a significant role. VCNS will be an LPSS.

- Instrument concepts need to be developed and demonstrated. We intend to convene a pair of workshops, a “one-two punch.” If sufficient interest in the science emerges from this workshop, we will convene another at a later time.

- No prototype of VCNS has existed or yet exists on which to demonstrate the moderator or the instrument concepts. LENS may serve in this essential role, as might a modification of IPNS.
VCNS: Design Challenges

- The main problem to be overcome in the design is to reduce the nuclear heating (neutron and $\gamma$) in the moderator medium while maintaining a high neutron flux in the moderator. The fundamental constraints are the low heat transport rates and low heat capacities of cryogenic materials.

- We have already reasonable assurance that the heat can be carried away in a time-average sense from the moderating material (tentatively, $D_2O$ ice or Be metal) by flowing L-He.

- A new aspect of the problem is that the instantaneous heating of the moderating medium can raise the temperature during the pulse to unacceptable levels.
VCNS: Design Approach

• Because nuclear heating (fast n and $\gamma$ from the source) decreases exponentially with distance from the source region, while neutrons, in the absence of absorption, are preserved in slowing-down, we expect to find a large radius at which the heating is acceptable and the cold neutron flux is as large as possible.

• The source power in this approach is an adjustable parameter.

• This is a departure from convention in neutron facility design, but has some similarities to the thermal columns of the “Atoms for Peace” reactors of the 1950s.
VCNS: Optimization

• The parameter to be optimized is the ratio of cold neutron flux to nuclear heating in the moderator. This ratio improves with distance from the source, but at the sacrifice of the ratio of cold neutron flux to source power.

• Moderator heating at large distances from the source is predominantly due to capture gamma rays that originate in the shielding material.

• Optimizable parameters are the distance of the moderator from the source, the choice and layering of shielding materials, and the source power and pulsing frequency. The tool is MCNPX.
What We Hope To Do

• Uncover scientific applications for VCNS
• Develop instrument ideas for VCNS that serve the science
• Compile a proceedings of this Workshop (see 1973 model)
• Apply for funding to carry on
• Extend technical studies of the source and instruments
Requests to the participants

- Prepared talks, please leave Powerpoint overheads with Nicole Green
- We will name discussion leaders and ANL assistants —
- Leaders please prepare brief summary presentations
- Please write up notes of discussions, ready in ~ 3 weeks.
The figure shows the slowing-down density, $q(r,E)$, of neutrons from a point source in an infinite medium of bismuth, calculated from classical theory. Slow ($\sim 1.\text{ meV}$) neutrons survive at large radii, while energetic neutrons that contribute to nuclear heating diminish substantially beyond radii of about 1 meter.

The flux per unit energy is related to the slowing-down density as $\Phi(r,E) = q(r,E)/\xi \Sigma_s E$. 

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VCNS: Gamma Rays

Gamma rays carry off on the order of 10% of the proton beam energy. The target itself and the primary shield reduce to insignificance the contribution of those to the the heating (dose rate) in the moderator beyond about 0.5 m from the source. This seems to dictate use of high-Z shielding, Pb or Bi, which are also effective fast neutron shielding materials.

An opportunity to reduce capture gamma rays from the shielding seems to lie in shielding with “radiogenic lead,” some varieties of which have lower slow- and resonance-capture cross sections than natural lead or of bismuth.
Relevant Activities Elsewhere

ISIS TS-II
— optimization of TMRS using MCNP imbedded in an optimization routine.

ESS
— development of ideas for instruments for long-pulse neutron sources.

PSI Spallation Ultra-Cold Neutron Source (SUNS)
— development of scattering data for very cold moderator materials.

Biennial meetings on UCN and cold neutron source technology are held in Russia (next meeting, St. Petersburg, July, 2005)
— general information and review.
VCNS MCNPX Model A (Cylindrically Symmetric)

- Moderator
- Target Bismuth
- Water Coolant/Premoderator
- Neutron Beam Channel
- Shield
- Proton Beam

Approximately 1 meter
Neutron Intensity from D$_2$O Ice Moderator
Model A

- Neutron energy (eV)
- Spectral intensity $i(E)$ (n/s-sr-mA)

D$_2$O, 2.17 K
Neutron Pulse Shapes from D$_2$O Ice Moderator Model A

- For $E_n = 0.2$ meV
- For $E_n = 0.1$ meV
VCNS MCNPX Model B
(Cylindrically Symmetric)

- Outer Shield, Reflector
- Inner Shield
- Proton Beam
- Water Coolant
- Bismuth Target
- Solid CH$_4$ Premoderator
- Moderator
- ~ 1 meter
VCNS MCNPX Model B: Results

- bismuth
- bismuth + 15 cm Be + 2 cm CH4
- bismuth + Be + 2cm CH4
- bismuth, 82 cm

Graph showing the ratio of thermal flux to heat in moderator vs. material thickness (cm).
VCNS MCNPX Model C
(Cylindrically Symmetric)

Bismuth
Inner
Shield

D$_2$O
Coolant

Bismuth
Target

Moderator

~ 1 meter

Proton Beam
VCNS MCNPX Model C: Results

![Graph showing the relationship between moderator average heating (mW/cc) and bismuth thickness (cm). The graph includes a linear trend line and a best-fit exponential line given by $\exp(-0.0224r)/r^2$.]

- **Simulation results**
- $\exp(-0.0224r)/r^2$
The figure shows the data of Long and Kemp, presumably $\text{D}_2\text{O}$ ice1h (frozen from the liquid), which extend to temperatures just low enough to justify extrapolation to the lower temperatures of interest to us.

Because the low-temperature limit of the Debye expression for the lattice specific heat of insulators indicates that $C_p$ is proportional to $T^3$, we have extrapolated accordingly as the figure shows.

(1 cal/mole = 0.2088 joules/gm)
VCNS Accelerator System

• We have worked out the conceptual design of an accelerator system to drive the VCNS.
  – 1-GeV proton linac, 300 kW time-average beam power.
  – Instantaneous current, 75 mA.
  – Pulse length, 4 msec, Pulsing frequency, 1 Hz.

• The linac components are ones common in modern high-power proton linac technology.

• The VCNS will complement the capabilities of the SNS in the very cold neutron regime. The SNS accelerator system is not capable of driving the conceived VCNS.
**BASIC CAVITY TYPES IN VCNS LINAC**

<table>
<thead>
<tr>
<th>CAVITY TYPES</th>
<th>Frequency MHz</th>
<th># OF CAVITIES</th>
<th>Ein MeV</th>
<th>Eout MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Room Temperature Triple Spoke</td>
<td>325</td>
<td>20</td>
<td>3</td>
<td>15</td>
</tr>
<tr>
<td>Superconduction Single Spoke</td>
<td>325</td>
<td>30</td>
<td>15</td>
<td>40</td>
</tr>
<tr>
<td>Superconduction Double Spoke</td>
<td>325</td>
<td>30</td>
<td>40</td>
<td>112</td>
</tr>
<tr>
<td>Superconduction Triple Spoke</td>
<td>325</td>
<td>44</td>
<td>112</td>
<td>400</td>
</tr>
<tr>
<td>Superconducting Elliptical 0.81 b</td>
<td>1300</td>
<td>48</td>
<td>400</td>
<td>1044</td>
</tr>
</tbody>
</table>

\[
f(\text{MHz}) = 325 \quad \quad 1300\]

![Diagram showing various components and their corresponding W(MeV) values]
VCNS Accelerator System

• The accelerator and target systems and the experiment area could fit into available space near Argonne’s 362 building, which could house the operations scientific staff.

• A very preliminary estimate of the cost of the installation is $500-600 M for the accelerator systems, $100 M for the target systems and the experimental area.
VCNS: Summary Remarks

• Efforts to date have largely been devoted to working out a feasible design for the VCNS accelerator system, and to scoping studies on the target/moderator system neutronics, all done on an as-time-is-available basis.

• The neutronics analysis and optimization requires much more work and innovation.

• The science case needs fleshing out both to show that there is a basis for the facility and to provide motivation and purpose for neutron scattering instrument concept development.

• If the project is ever to fly, feasibility needs to be demonstrated in a prototype; LENS may serve in that role.

• The enterprise will soon need LDRD funding in order to progress.
End of presentation
extra materials follow
VCNS: Challenges

• Neutronic simulations require scattering kernels that don’t exist for the temperatures of interest—developing these kernels requires considerable effort. We are in touch with workers in the laboratories where work is going on with this goal. The MCNPX code requires modifications to enable calculations in the very low temperature regime. Meanwhile, we do as well as we can with approximate descriptions of the scattering.

• Data on low-temperature thermal conductivities and specific heats of candidate moderator materials are sparse, yet essential to evaluating static and dynamic effects of moderator heating. We need more data than are now in hand.

• Heat transfer calculations for L-He cooling is a special field. We have gained the assistance of a specialist, S. Van Sciver, FSU.
VCNS: Challenges, more

- There is little or no experience with neutron scattering instruments suitable for the expected scientific applications and for use of very cold neutrons in the long-pulse mode.

- Concepts need to be developed and demonstrated. We intend to convene a pair of workshops, a “one-two punch,” to address these questions in collaboration with LENS, Indiana U. The outcome of these workshops will almost certainly affect the accelerator parameters and the engineering design.

- No prototype of VCNS has existed or yet exists on which to demonstrate the moderator or the instrument concepts. LENS may serve in this essential role, as might a modification of IPNS.
Radiogenic Lead

• All natural lead (204,206,207,208) is either “primordial” (i.e. produced directly in the supernova 4.56 Gy ago), or “radiogenic,” i.e. the stable products of the three natural actinide decay chains. The Th-232 chain gives Pb-208; the U-238 chain gives Pb-206; the U-235 chain gives Pb-207. Lead-204 is only primordial.

• Different U and Th mines produce different isotopic ratios of lead as byproduct, which are advantageously depleted in the neutron-capturing isotopes $^{204}\text{Pb}$ and $^{207}\text{Pb}$.

• For example, years ago, two varieties of radiogenic lead were feedstocks for ORNL calutron production of isotope-separated reference lead materials. The table that follows compares the 2200-m/sec capture cross sections and the resonance capture integrals of the isotopes and example mixtures.
VCNS: Gamma Rays, Radiogenic Lead

Gamma rays generated in the shielding dominate the heat production in the moderator. Radiogenic lead is available in isotopic compositions that reduce the capture rate in the shield.

<table>
<thead>
<tr>
<th>A</th>
<th>$\sigma_\gamma$, mb</th>
<th>I, mb</th>
<th>Primordial Lead Standard Composition</th>
<th>Radiogenic Lead High-206 Lead</th>
<th>Radiogenic Lead High-208 Lead</th>
</tr>
</thead>
<tbody>
<tr>
<td>204</td>
<td>661.</td>
<td>1700.</td>
<td>f, %</td>
<td>f $\sigma_\gamma$</td>
<td>f I</td>
</tr>
<tr>
<td>206</td>
<td>30.5</td>
<td>200.</td>
<td>1.4</td>
<td>9.2</td>
<td>24.</td>
</tr>
<tr>
<td>207</td>
<td>709.</td>
<td>400.</td>
<td>22.1</td>
<td>156.</td>
<td>88.</td>
</tr>
<tr>
<td>208</td>
<td>0.5</td>
<td>2.0</td>
<td>52.4</td>
<td>0.26</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Averages

<table>
<thead>
<tr>
<th></th>
<th>$\sigma_\gamma$</th>
<th>I</th>
<th>$\sigma_\gamma$</th>
<th>I</th>
<th>$\sigma_\gamma$</th>
<th>I</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radiogenic</td>
<td>20.9</td>
<td>73.2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Bismuth (monoisotopic), $\sigma_\gamma = 34$. Mb, I = 190 mb, is much superior to standard lead. However, the “high-208” radiogenic lead is better still.

The average gamma energies emitted per capture are 5408, 6714, and 4663 keV for the three varieties of Pb, and 4604 keV for Bi.
Neutron Flux Profile inside D$_2$O Ice Moderator Model A
Neutron Pulse Shapes from D$_2$O Ice Moderator
Model A

\[ E_n = 1.0 \text{ meV} \]

\[ E_n = 0.5 \text{ meV} \]
Heat Capacities of D$_2$O and Be: Heating

If a short power pulse deposits heat $\Delta Q$ per gram in the moderator, initially at temperature $T_1$, the material heats up immediately to a temperature $T_2$ such that $\Delta H(T_2, T_1) = \Delta Q$, where $\Delta H$ is the difference in enthalpy between temperatures $T_2$ and $T_1$),

$$\Delta H(T_2, T_1) = \int_{T_1}^{T_2} C(T)\,dT = 4.64 \times 10^{-6} (T_2^4 - T_1^4) \text{ j/gm for D}_2\text{O}.$$

If we say $T_1 = 2K$ and insist that $T_2$ remain less than $4K$, then $\Delta H = 1.14 \times 10^{-6} \text{ j/gm}$ and $\Delta Q$ must be $\Delta Q < \Delta H = 1.14 \times 10^{-6} \text{ j/gm}$, a very conservative assumption that represents our goal.

By contrast, the specific heat of beryllium (a metal) is $C(T) = 2.5 \times 10^{-5} \text{ T j/gm-K}$, so $\Delta H(T_2, T_1) = 1.5 \times 10^{-4} \text{ j/gm}$.

Beryllium may provide a needed heat capacity advantage over D$_2$O, although D$_2$O and D$_2$ are, we expect, better moderators.
VCNS Monte Carlo Results
first round

Volume- and time-averaged thermal neutron flux in moderator vs. Bi radius
VCNS model C, 300 kW beam power

Time average heating density vs. Bi radius
VCNS Model C, 300 kW proton beam
VCNS Monte Carlo Results

Ratio of time-average thermal neutron flux to time-average heating density vs. Bi radius
VCNS Model C, 300 kW beam power

Heat deposited in moderator per pulse for various frequencies vs. Bi radius
VCNS Model C, 300 kW beam power
Peak and time average fluxes in Be and D\textsubscript{2}O moderators
VCNS Model C, 300 kW beam power