

# Workshop on Present Status and Future of Very Cold Neutron Applications Paul Scherrer Institute 13, 14 February 2006



Prospects for a Very Cold Neutron Source at  
Argonne National Laboratory

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# VCNS: Motivation

The practical motivation for our 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.
- Preliminary studies lead to Pb as target material and as fast-neutron shield, and to a 2-to-4 K pebble-bed of D<sub>2</sub>O ice, solid D<sub>2</sub> or CD<sub>4</sub> moderator cooled by flowing L-He.
- The response time of a 2-K D<sub>2</sub>O moderator, about 4 msec, indicates a “long-pulse” operating mode. Long-wavelength ( $\sim 20$  Å) neutrons require long interpulse intervals, therefore a low pulsing frequency.
- We assume 1.5-MW proton beam, 4-msec pulse width and 5-Hz pulsing frequency, indicating a linac accelerator driver.

# For Reference

The energy of 2.2 K neutrons is  $190 \mu\text{eV}$ ;

The wavelength is  $20.8 \text{ \AA}$ ;

The speed is  $190. \text{ m/sec}$ .

# VCNS: Safe Observations

- Production of large quantities of mm-scale, solid pellets ( $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{NH}_3$ ,  $\text{D}_2$ , ... ) is an established technology
- Target technology presents no overwhelming challenges.
- A prolific source of Very Cold Neutrons with wavelengths  $\sim 20 \text{ \AA}$ , energies  $\sim 100 \mu\text{eV}$  will serve applications in studies of large structures and slow motions: nanotechnology and biological sciences

# 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

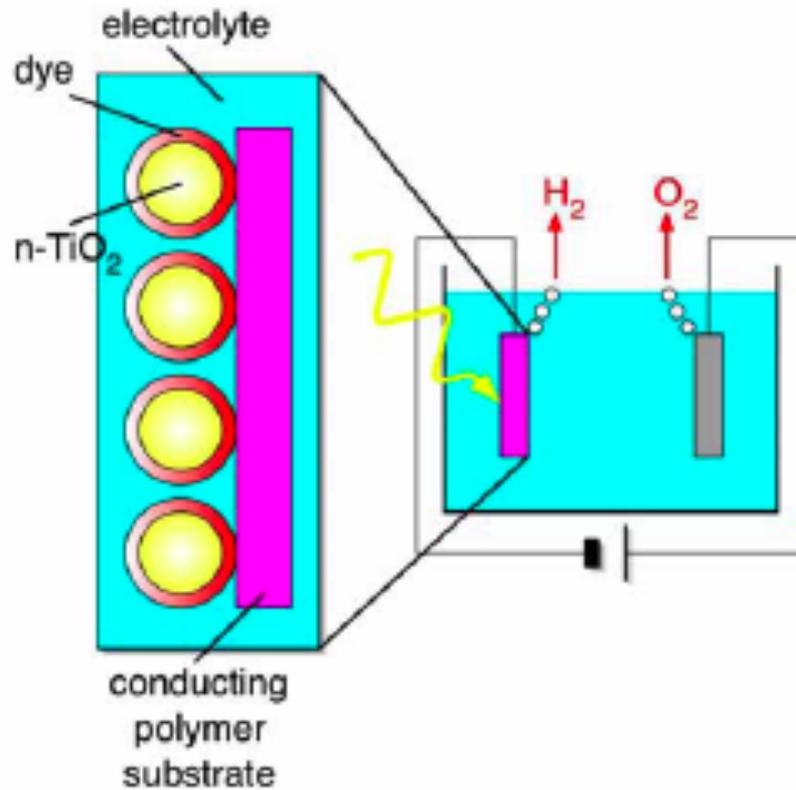
- There is little or no experience with neutron scattering instruments suitable for the expected scientific applications and for use of very cold neutrons in the long-pulse mode.
- Instruments are likely to rest heavily on neutron optical devices all of which work better at long than at short wavelengths. Beam modulation and spin-echo methods loom large.
- Concepts need to be developed and demonstrated. ANL convened a Workshop on Application of a VCNS held 21-24 August 2005. The proceedings will soon be published.
- No prototype of VCNS yet exists on which to demonstrate the target, moderator or the instrument concepts.

# VCNS Workshop



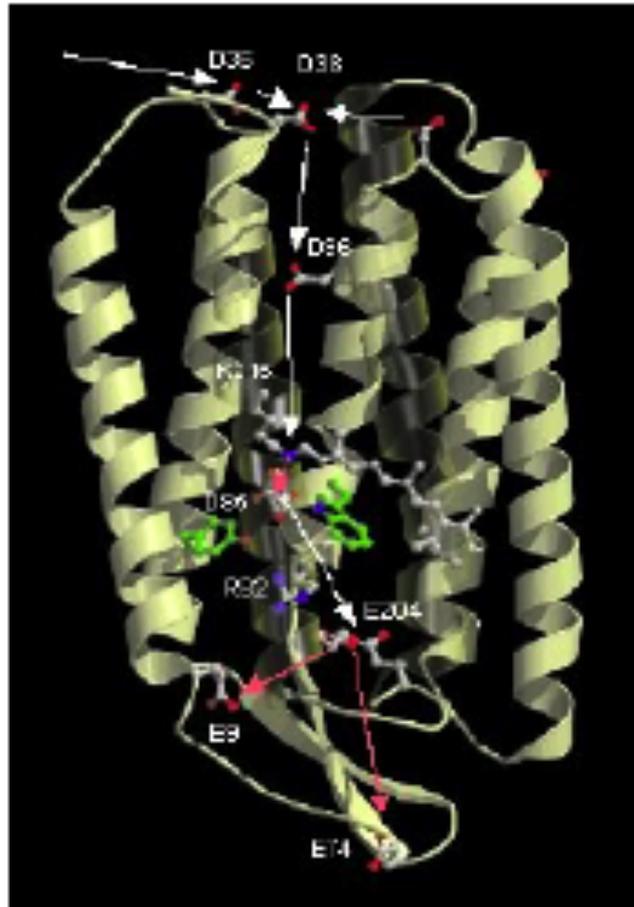
# VCNS Applications

## nanoscale-enhanced photocleavage of water



# VCNS Applications

## light-driven protein-based proton pump



# 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.
- A new (to SPSS aficionados) aspect of the problem is that the instantaneous heating of the moderating medium can raise the temperature during the pulse to unacceptable levels.

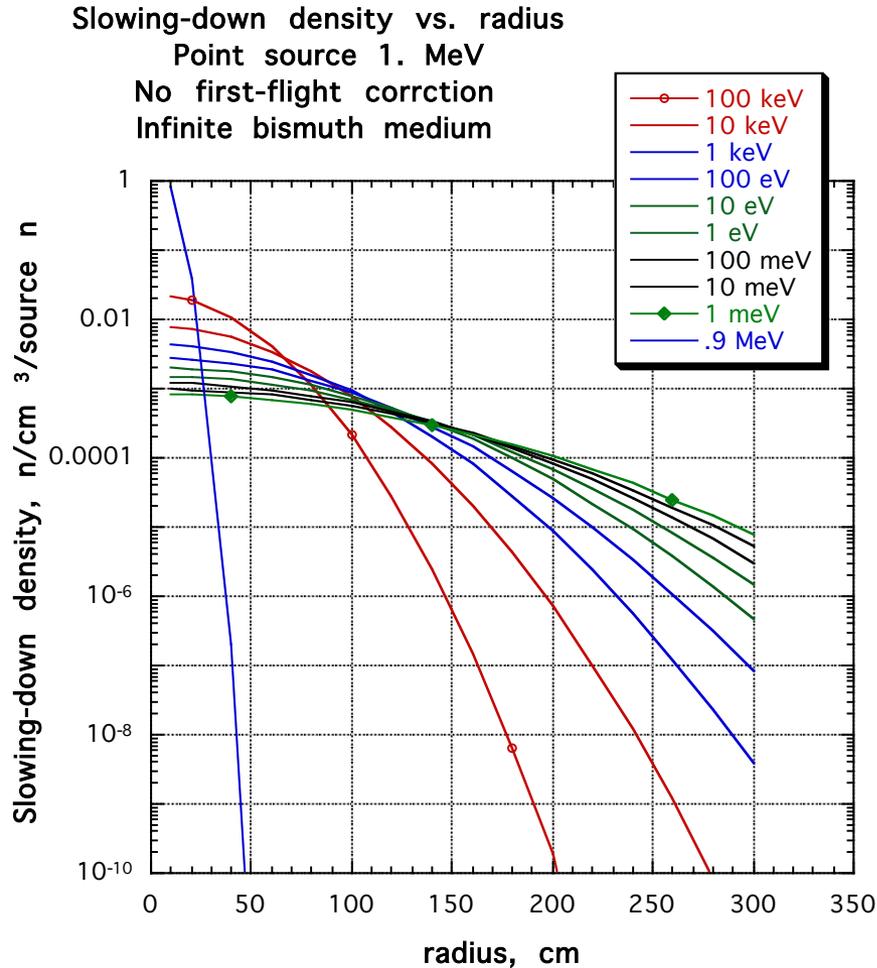
# VCNS: Design Approach

- 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.

# 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 ratio of cold neutron flux to source power.
- Moderator heating at large distances from the source seems to be 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.

# VCNS: Analytical Results



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 ( $\sim 1$  meV) neutrons survive at large radii, while fast neutrons and gammas 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  $\Phi(r,E) = q(r,E)/\xi\Sigma_s E$ .

# 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. E. g., the present meeting

Biennial meetings on UCN and cold neutron source technology are held in Russia (next meeting, St. Petersburg, July, 2005)

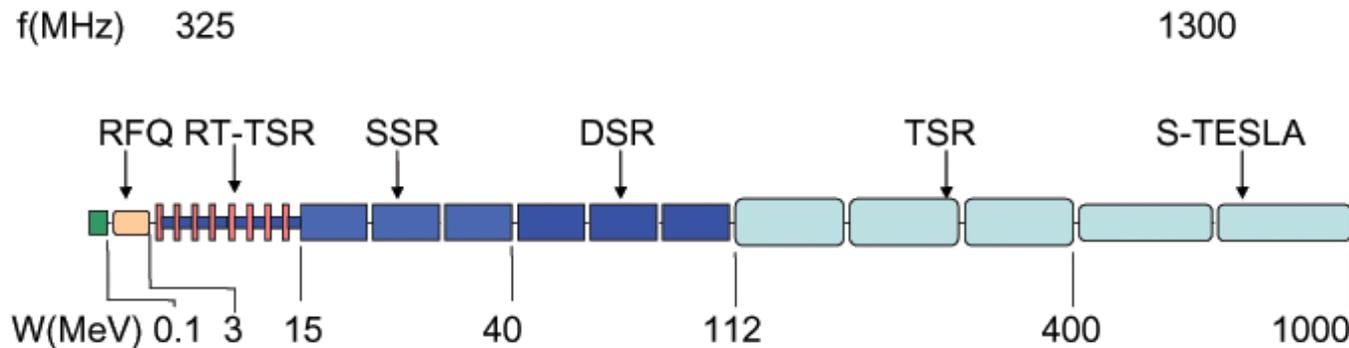
—general information and review.

# VCNS Accelerator System

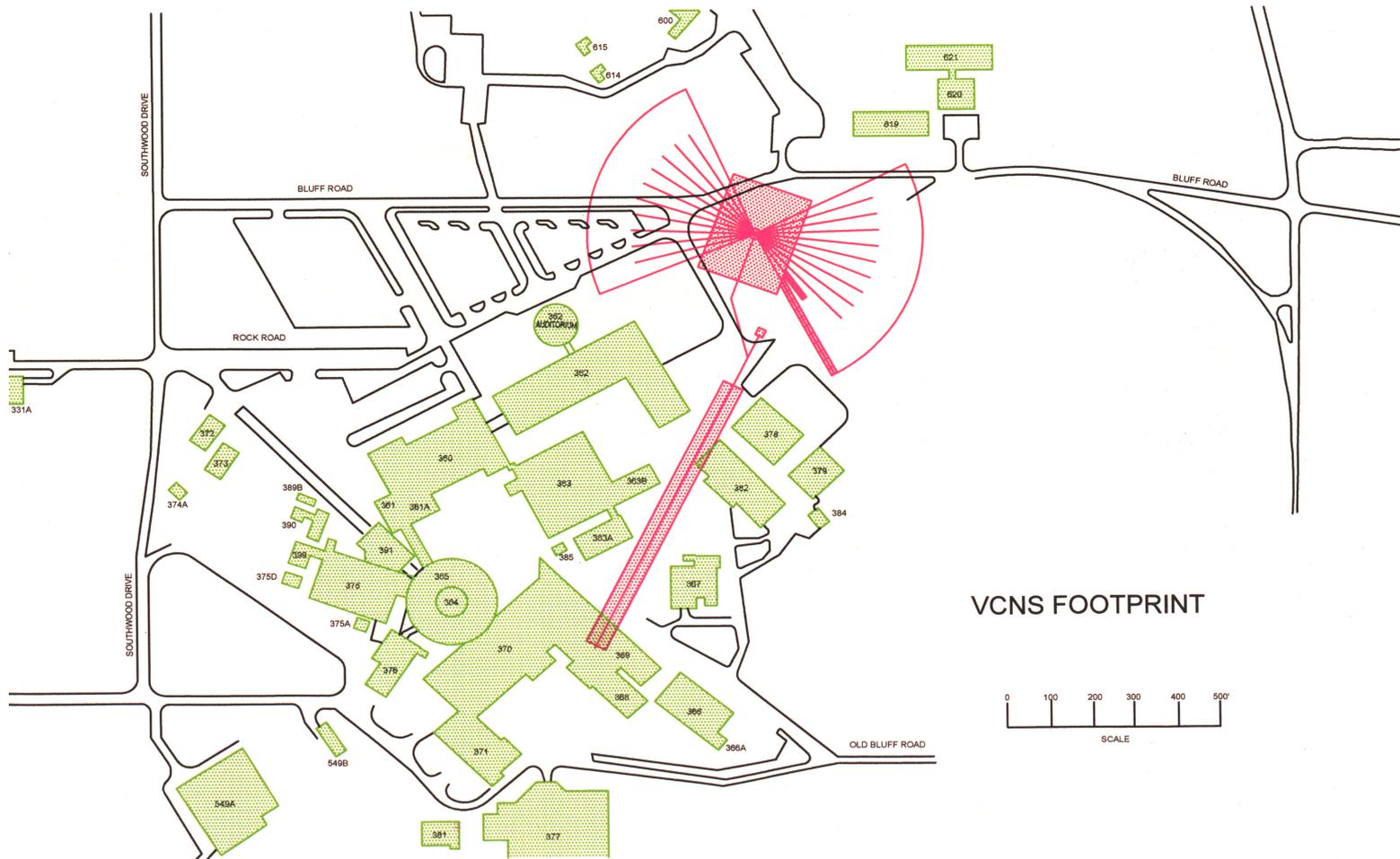
- We have worked out the conceptual design of an accelerator system to drive the VCNS.
  - 1-GeV proton linac, 1.5-MW time-average beam power.
  - Instantaneous current, 75 mA.
  - Pulse length, 4 msec, Pulsing frequency, 5 Hz.
- The linac components are ones common in modern high-power proton linac 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

CAVITY TYPES	Frequency MHz	# OF CAVITIES	Ein MeV	Eout MeV
Room Temperature Triple Spoke	325	20	3	15
Superconduction Single Spoke	325	30	15	40
Superconduction Double Spoke	325	30	40	112
Superconduction Triple Spoke	325	44	112	400
Superconducting Elliptical 0.81 b	1300	48	400	1044



# Possible Location for VCNS



# 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 or IPNS may serve in that role.
- We seek laboratory discretionary 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

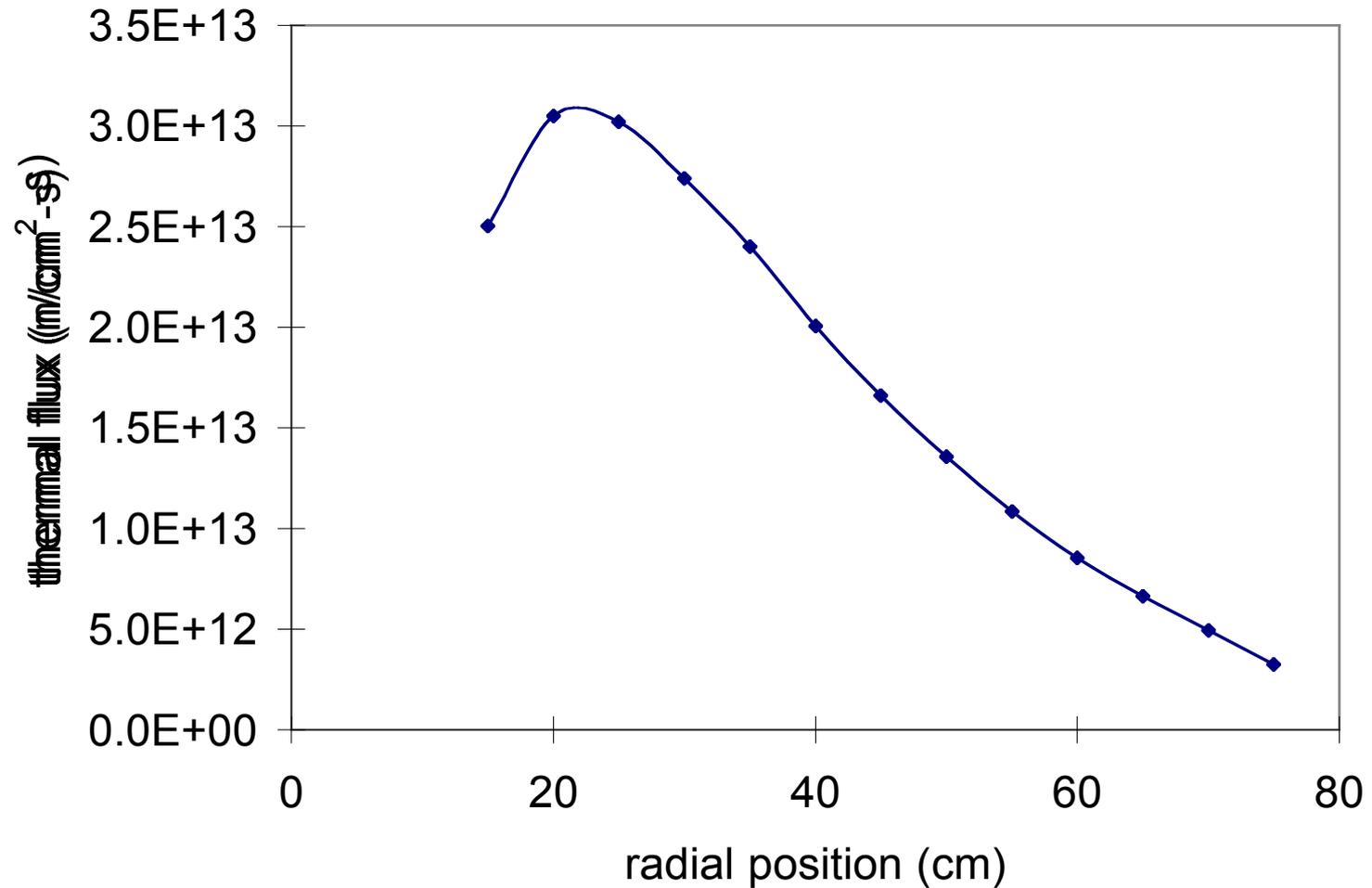
Gamma rays generated in the shielding dominate the heat production in the moderator. Radiogenic lead is available in isotopic compositions that reduce the capture rate in the shield.

A	$\sigma_\gamma$ , mb	I, mb	Primordial Lead Standard Composition			Radiogenic Lead High-206 Lead			Radiogenic Lead High-208 Lead		
			f, %	f $\sigma_\gamma$	f I	f, %	f $\sigma_\gamma$	f I	f, %	f $\sigma_\gamma$	f I
204	661.	1700.	1.4	9.2	24.	0.2	1.32	3.4	.024	.16	.41
206	30.5	200.	24.1	7.4	48.	87.8	26.8	176.	25.6	7.81	51.2
207	709.	400.	22.1	156.	88.	8.9	63.1	35.6	1.78	12.6	7.1
208	0.5	2.0	52.4	0.26	1.0	3.3	.017	.065	72.6	.36	1.45
Averages			$\sigma_\gamma$	I		$\sigma_\gamma$	I		$\sigma_\gamma$	I	
			173.	161.		91.2	218.		20.9	73.2	

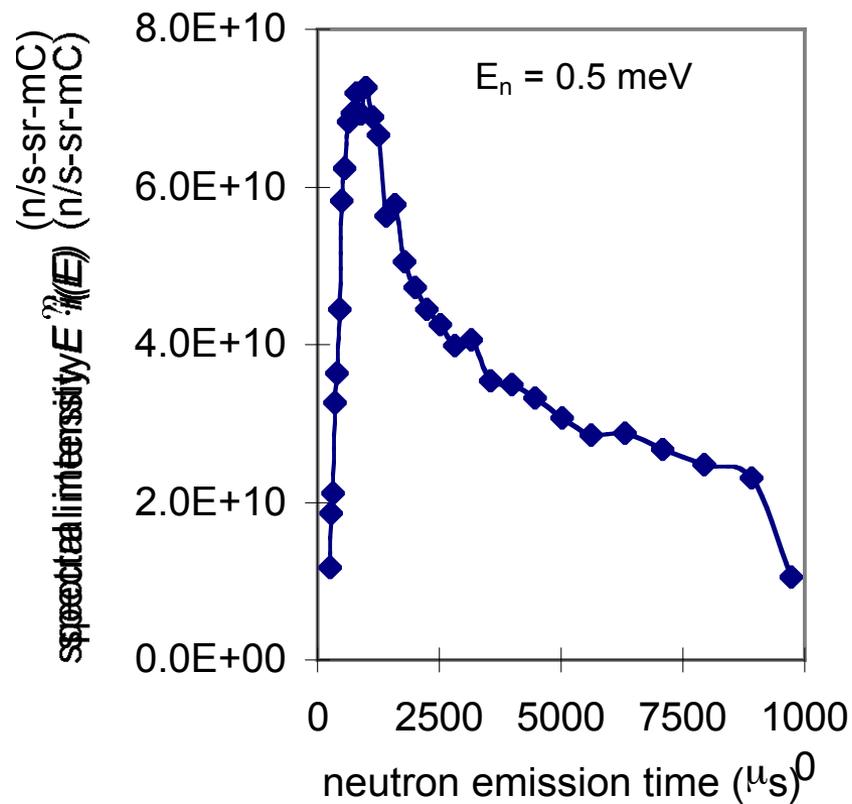
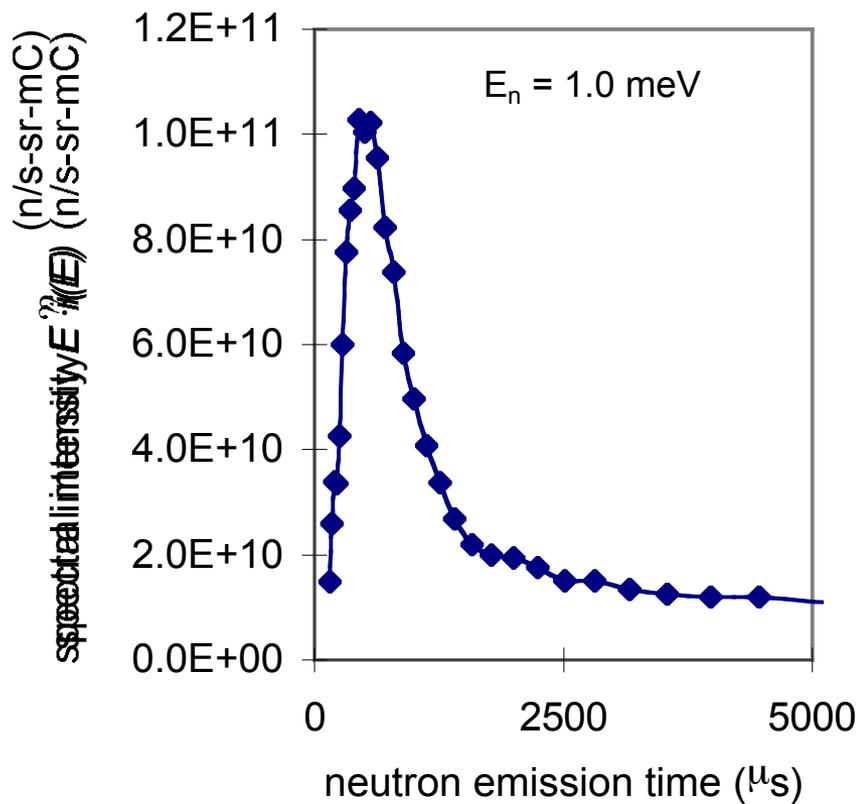
Bismuth (monoisotopic),  $\sigma_\gamma = 34$ . Mb, I = 190 mb, is much superior to standard lead. However, the “high-208” radiogenic lead is better still.

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<sub>2</sub>O Ice Moderator Model A



# Neutron Pulse Shapes from D<sub>2</sub>O Ice Moderator Model A



# Heat Capacities of D<sub>2</sub>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  $T_1 = 2\text{K}$  and insist that  $T_2$  remain less than  $4\text{K}$ , 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

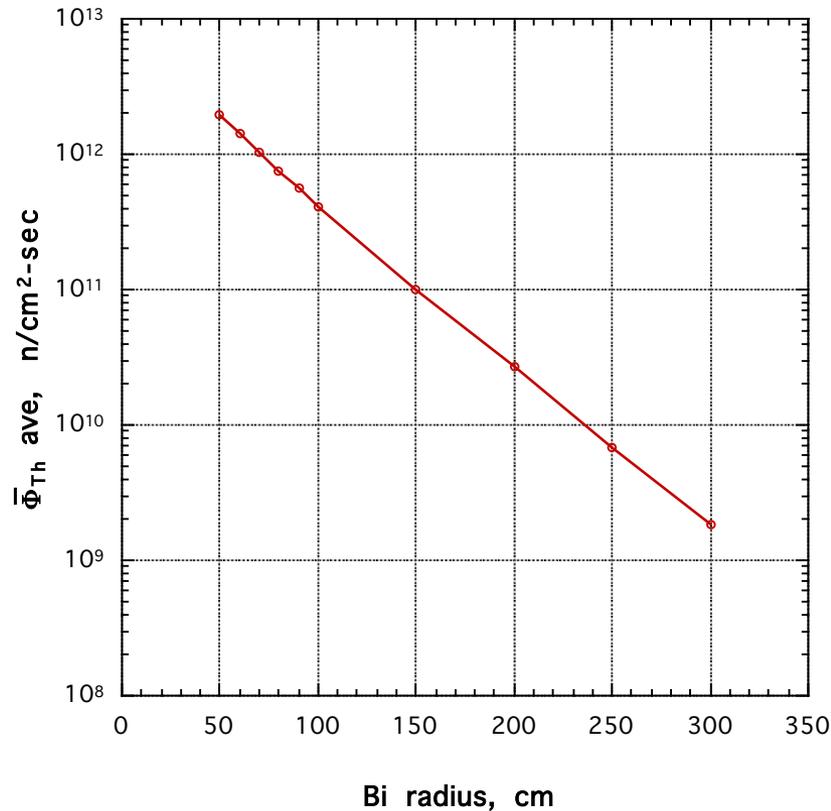
$$C(T) = 2.5 \times 10^{-5} T \text{ j/gm-K, so } \Delta H(T_2, T_1) = 1.5 \times 10^{-4} \text{ j/gm.}$$

Beryllium may provide a needed heat capacity advantage over D<sub>2</sub>O, although D<sub>2</sub>O and D<sub>2</sub> are, we expect, better moderators.

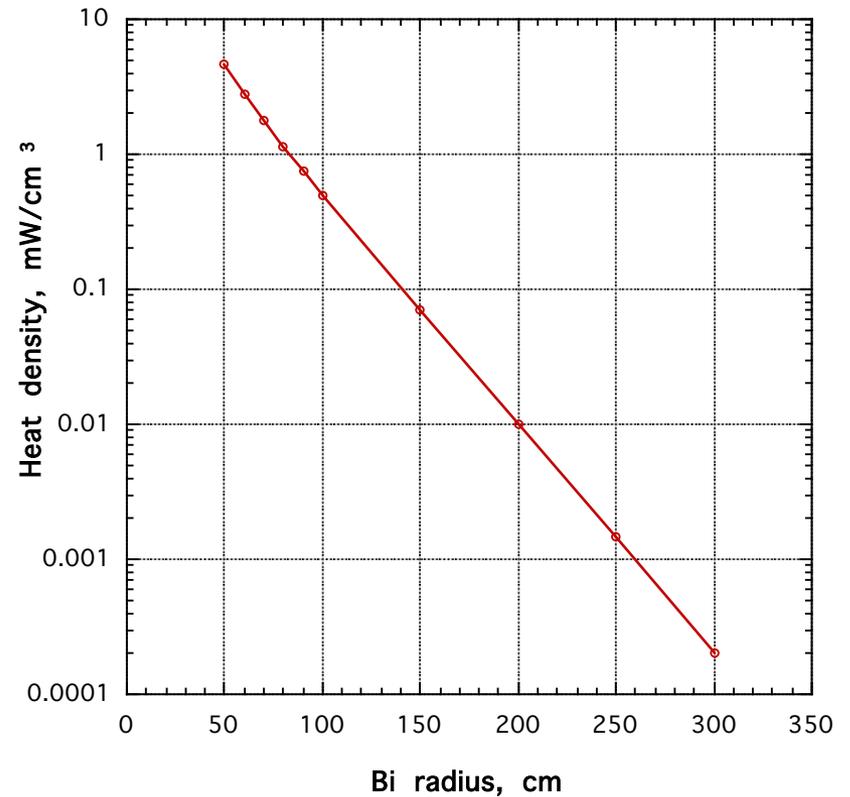
# VCNS Monte Carlo Results

## first round

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

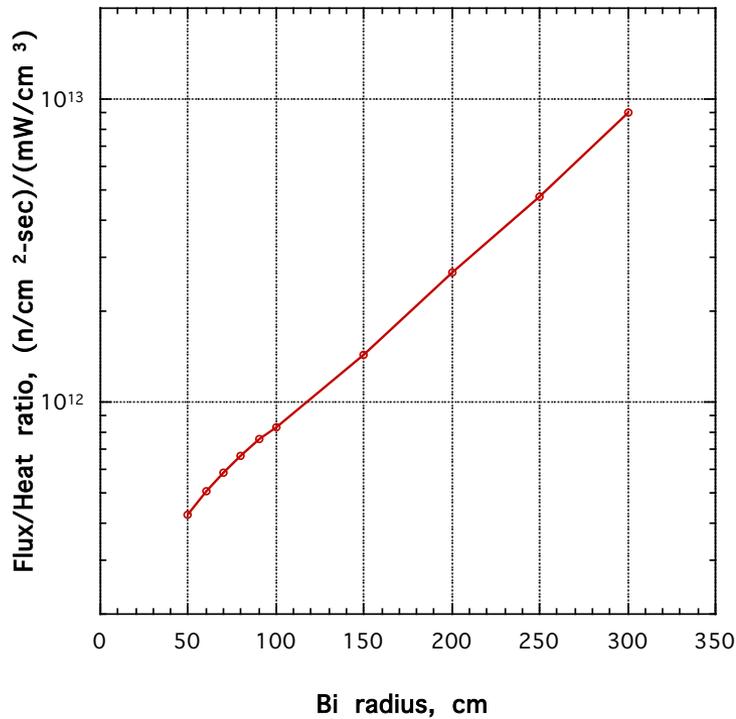


Time average heating density vs. Bi radius  
VCNS Model C, 300 kW proton beam

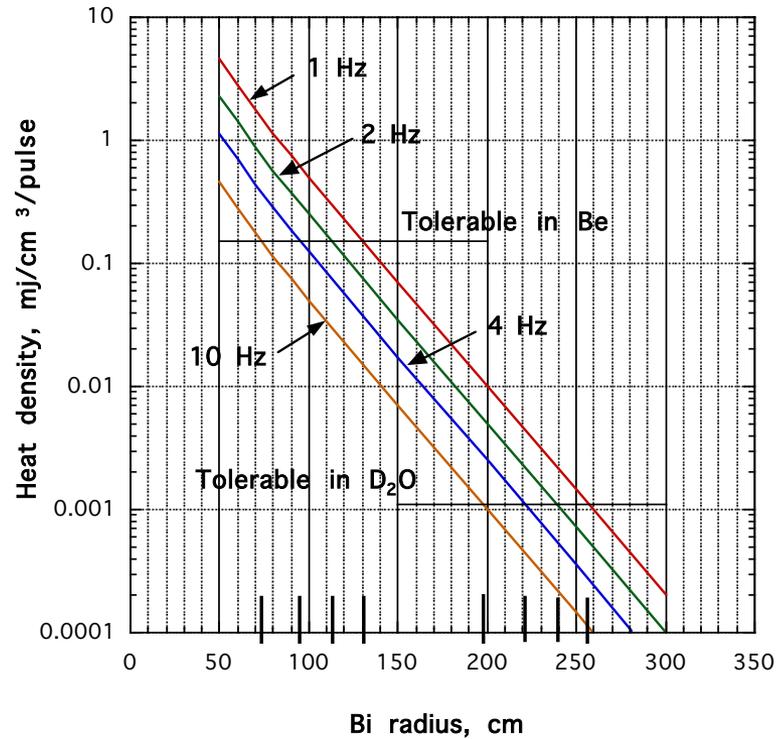


# VCNS Monte Carlo Results

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



# VCNS Monte Carlo Results

Peak and time average fluxes in Be and D<sub>2</sub>O moderators  
VCNS Model C, 300 kW beam power

