Prospects for a Very Cold Neutron Source

SNS
Oak Ridge National Laboratory
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(with lots of help from
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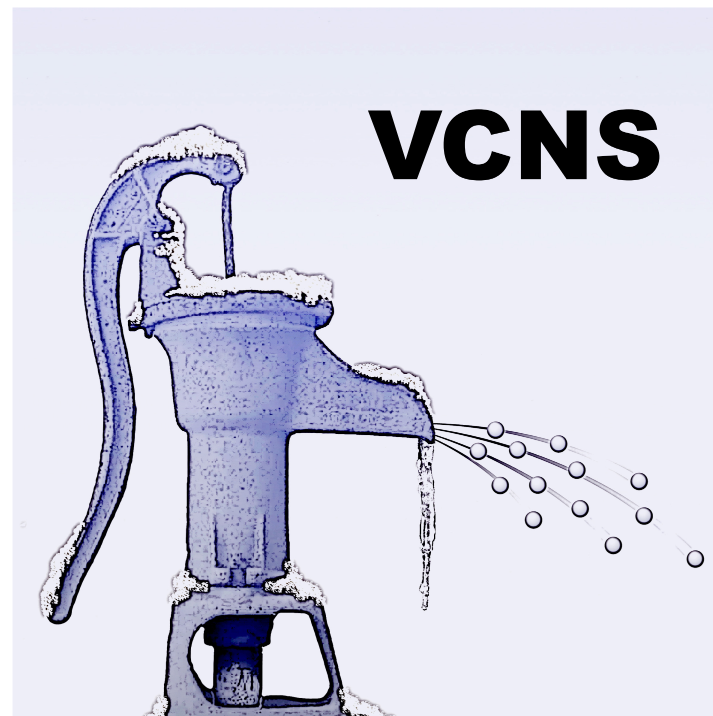


VCNS: Motivation

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_2O ice, solid D_2 or CD_4 moderator cooled by flowing L-He.
- The response time of a 2-K D_2O moderator, about 4 msec, indicates a “long-pulse” operating mode. Practical use of long-wavelength (~ 20 Å) neutrons requires 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.

Basic Quantities ("The Law of 2")

- At 2.2 K
  - Neutron energy ≈ 200 μeV (190 μeV)
  - Neutron wavelength ≈ 20 Å (20.8 Å)
  - Neutron velocity ≈ 200 m/s (190 m/s)

VCNS: Safe Observations

- Production of large quantities of mm-scale, solid pellets (CO_2, CH_4, NH_3, D_2, …) is an established technology
- Target technology presents no overwhelming challenges.
- A prolific source of Very Cold Neutrons with wavelengths ~ 20 Å, energies ~ 100 μeV 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.
- ANL convened a Workshop on Application of a VCNS held 21-24 August 2005. The proceedings will soon be published.
- 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.
- No prototype of VCNS yet exists on which to demonstrate the target, moderator or the instrument concepts.

VCNS: Design Challenges

- The main problem to be overcome in the design is to reduce the nuclear heating (neutron and γ) in the moderator medium while maintaining a high Very Cold neutron flux in the moderator. The fundamental constraints are the low heat transport rates and low heat capacities of cryogenic materials.
- A new (to present day 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.
- Need to avoid gamma heating of the moderator due to capture in the shielding, premoderator, reflector and moderator.

VCNS: Design Approach

- Because nuclear heating (fast n and γ 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.

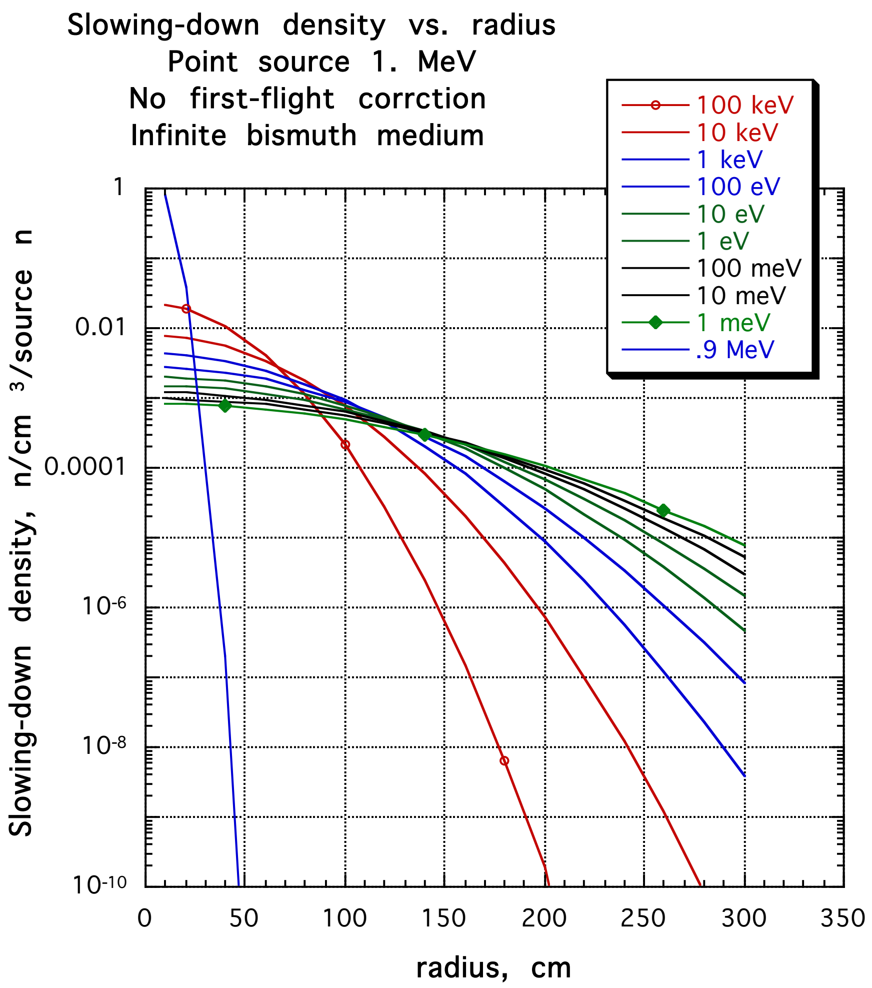
VCNS: Optimization

- 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.

Feasibility of the VCNS Concept

- Whether it is feasible to build a VCNS rest on three key questions
  - Are there scientific applications that would use these long-wavelength neutrons?
  - Can we build instruments that can take advantage of the unique characteristics of the proposed source?
  - Will the performance of the source in practical terms enable the kinds of research that we hope to attract?
- Studies of neutron source performance are the key to answering the last question and fundamental to answering the second question.
- Most of this presentation deals with the source.

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 (~ 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, operation of a UCN source. PSI hosted a workshop on Applications of VCNs in February 06.

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

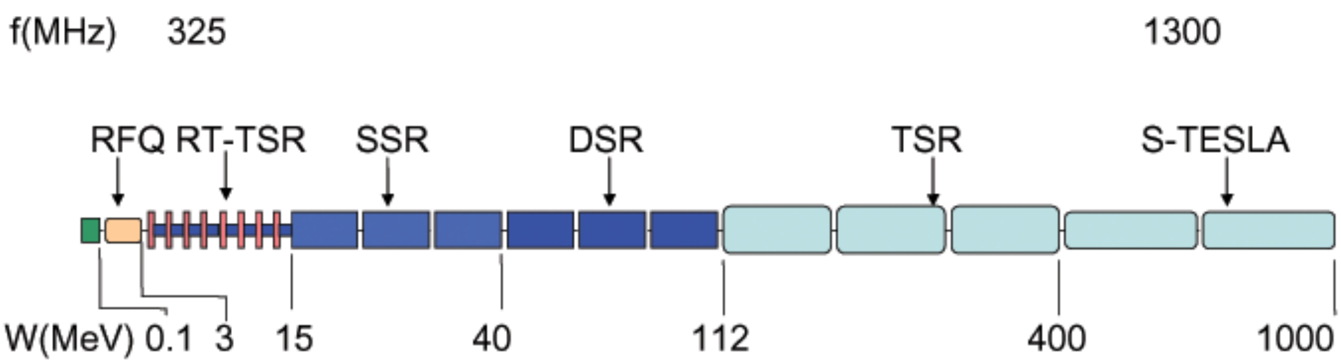
—general information and review.

VCNS Accelerator System

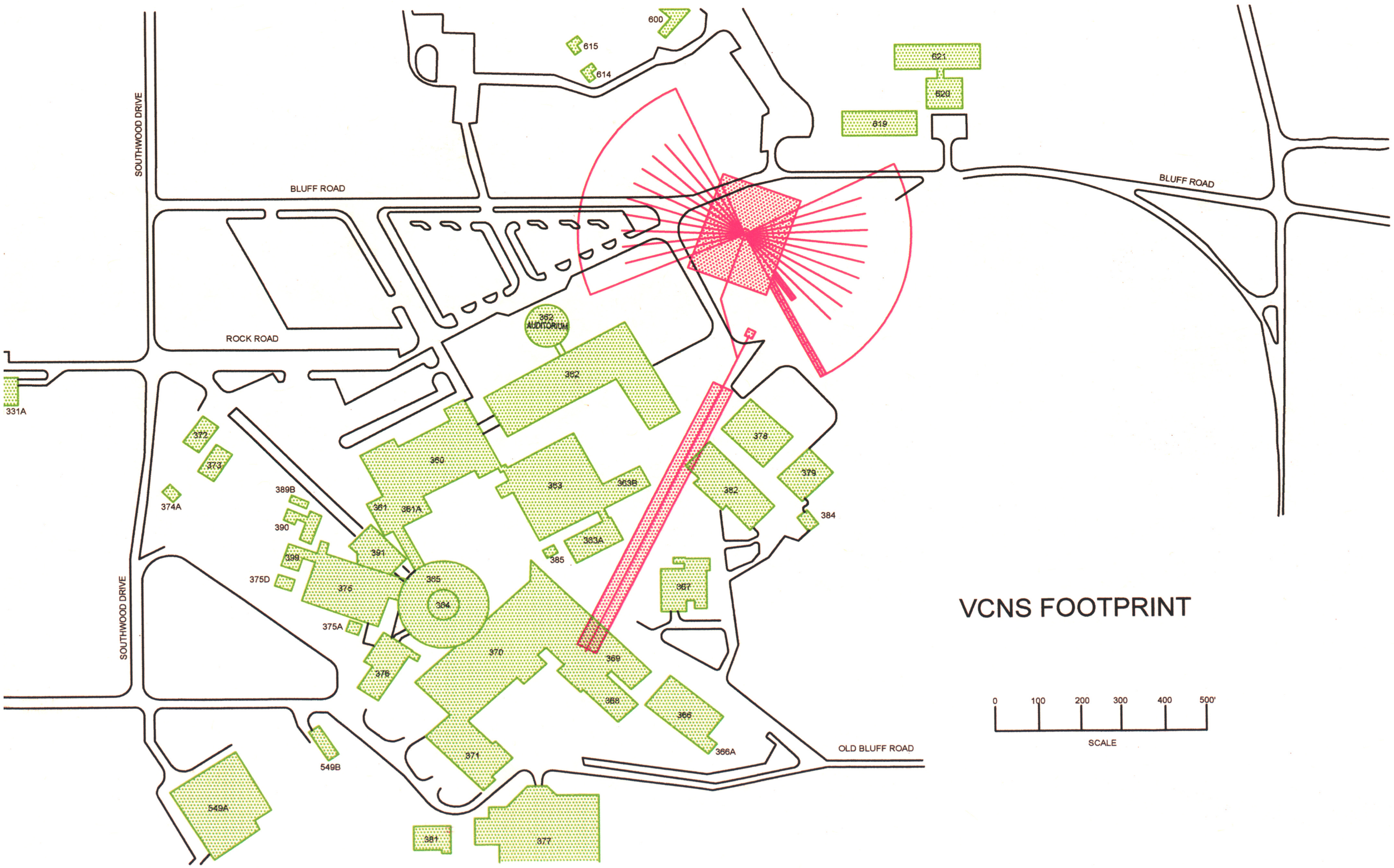
- We have worked out the conceptual design of an accelerator system to drive the VCNS.
  - 1-GeV proton linac
  - Instantaneous current, 75 mA.
  - Pulse length, 4 msec
  - Energy per pulse 300 kJ
  - Pulsing frequency, 5 Hz.
  - 1.5-MW time-average beam power.
- The linac components are ones common 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



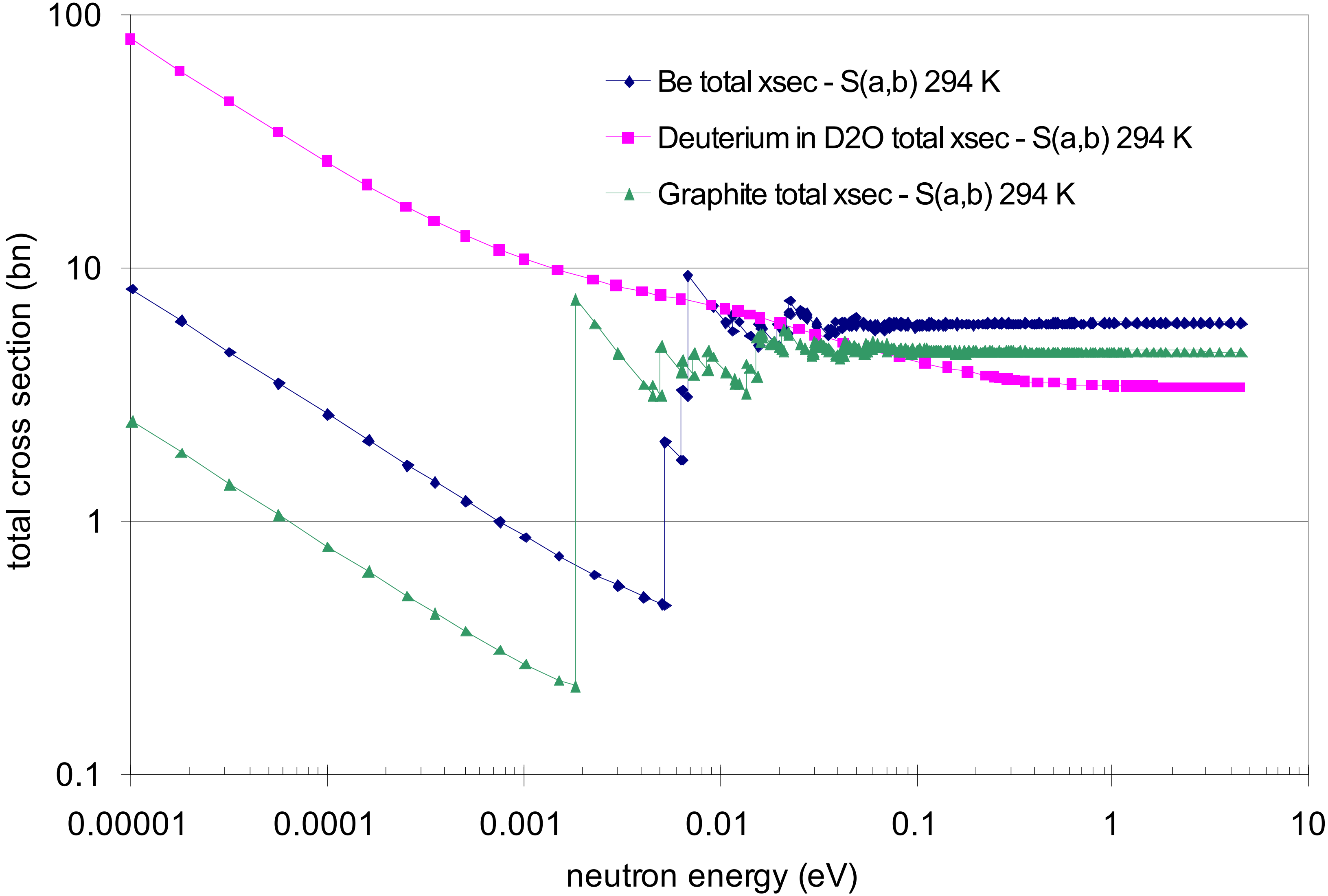
Possible Location for VCNS



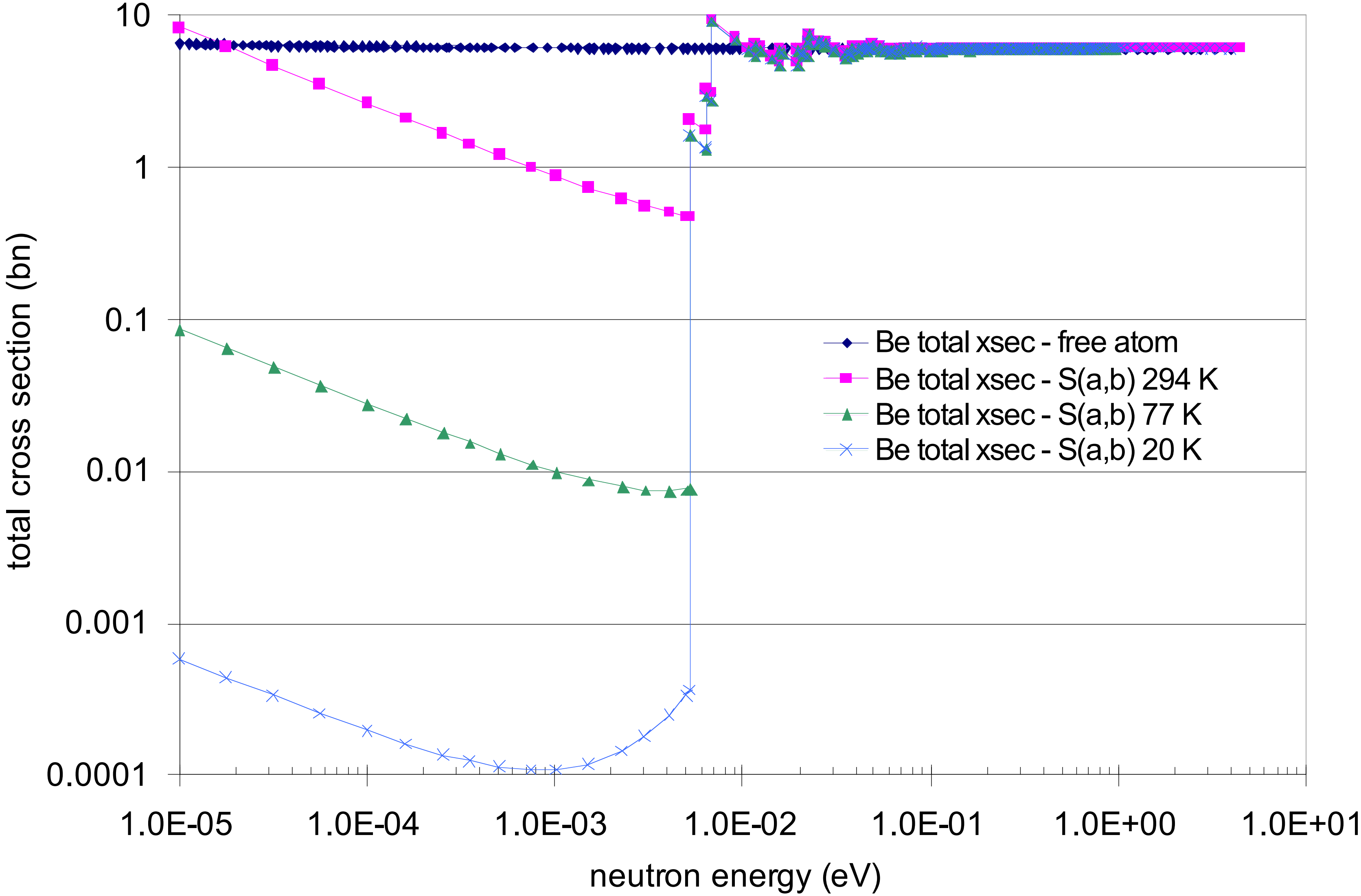
Materials Selection

- Target
  - Need high Z, low neutron absorption
  - Candidates: Hg (some n absorption), Bi (^{210}Po production), Pb
  - Radiogenic lead (low in ^{204}Pb, ^{207}Pb) could reduce moderator heating due to gamma generation
- Warm moderator
  - D_2O (H_2O neutron absorption much higher)
  - Beryllium, graphite, lead?
- Cold/Ultra-cold moderator
  - Rely on D (D_2, D_2O, CD_4, etc.) rather than H
  - Need a material with incoherent scattering at low temperatures & neutron energies
  - Be, graphite (Bragg edges make these poor choices)

Cross Sections for Candidate Moderators



Thermal Cross Sections – Beryllium



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}Pb and ^{207}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.

			Primordial Lead Standard Composition			Radiogenic Lead High-206 Lead			Radiogenic Lead High-208 Lead		
A	σ_γ, mb	I, mb	f, %	f σ_γ	f I	f, %	f σ_γ	f I	f, %	f σ_γ	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
				σ_γ	I		σ_γ	I		σ_γ	I
Averages				173.	161.		91.2	218.		20.9	73.2

Bismuth (monoisotopic), σ_γ = 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.

Heat Capacities of D_2O and Be: Heating

If a short power pulse deposits heat ΔQ 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 ΔH is the difference in enthalpy between temperatures T_2 and T_1),

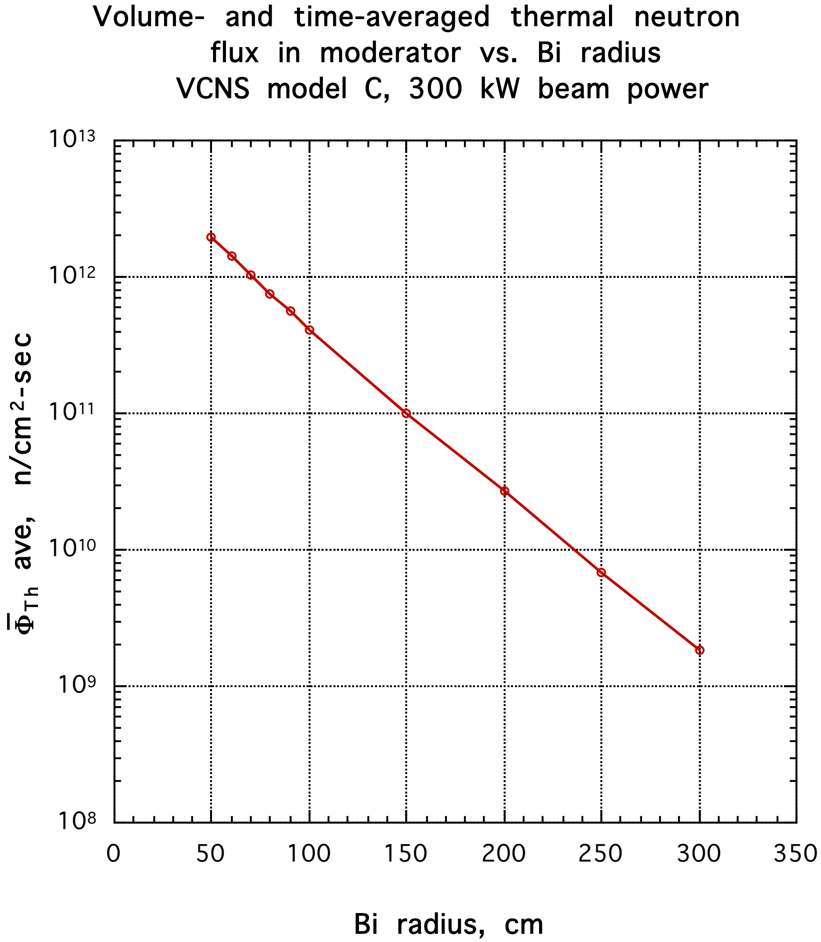
$$\Delta H(T_2, T_1) = \int_{T1}^{T2} C(T)dT = 4.64 \times 10^{-6}(T_2^4 - T_1^4) \text{ j/gm for } D_2O.$$

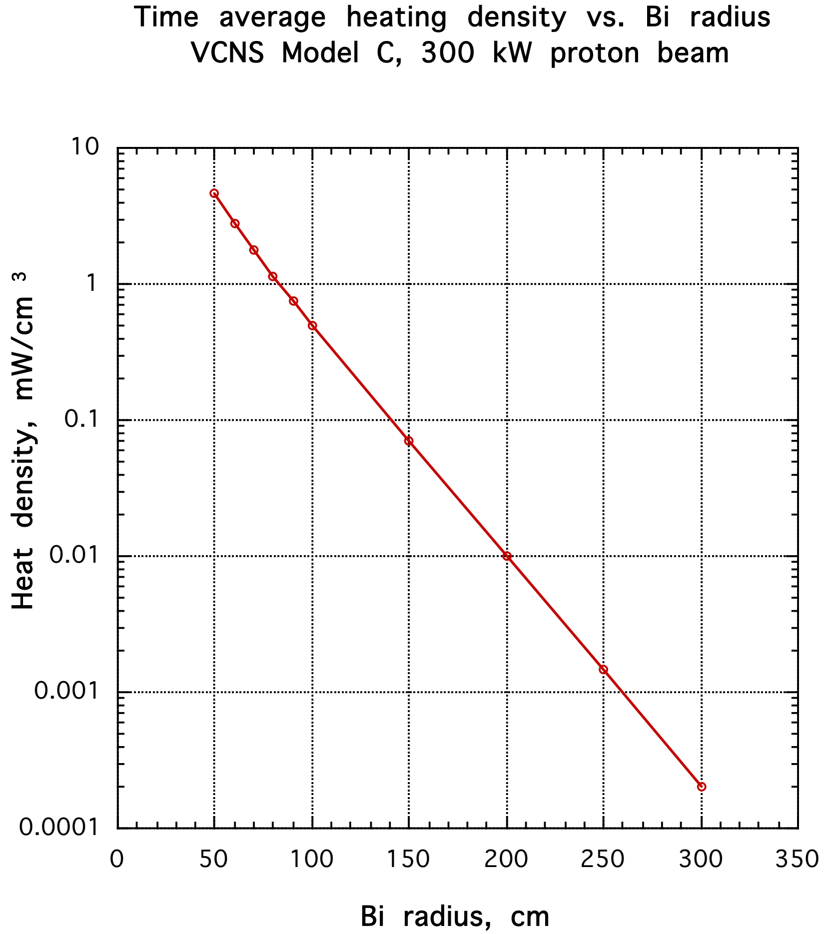
If we say $T_1 = 2K$ and insist that T_2 remain less than 4K, then $\Delta H = 1.14 \times 10^{-6}$j/gm and ΔQ must be $\Delta Q < \Delta H = 1.14 \times 10^{-6}$j/gm, a very conservative assumption that represents our goal.

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

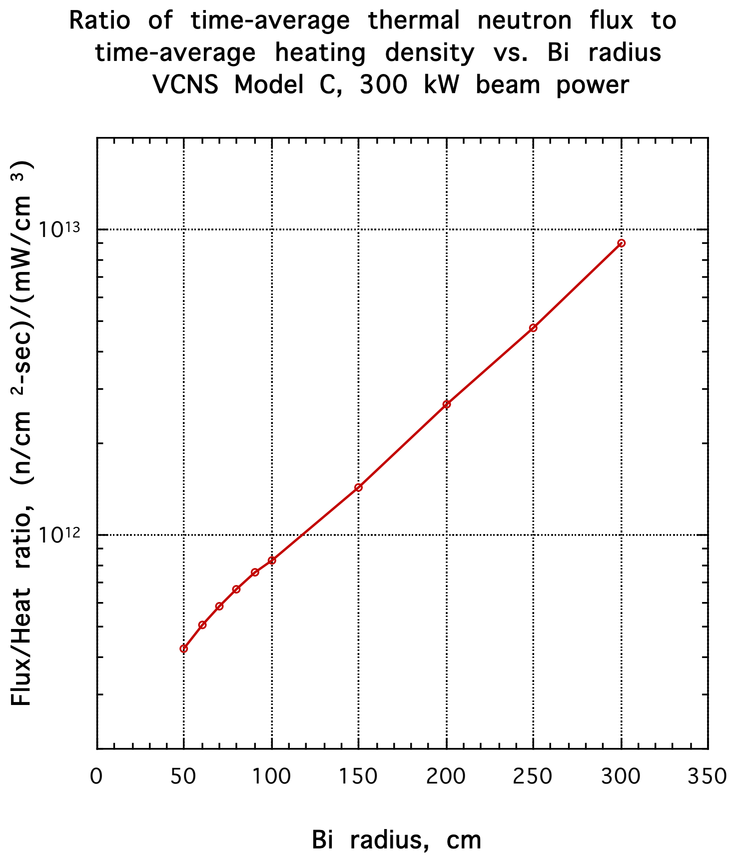
Beryllium may provide a needed heat capacity advantage over D_2O, although D_2O and D_2 are, we expect, better moderators.

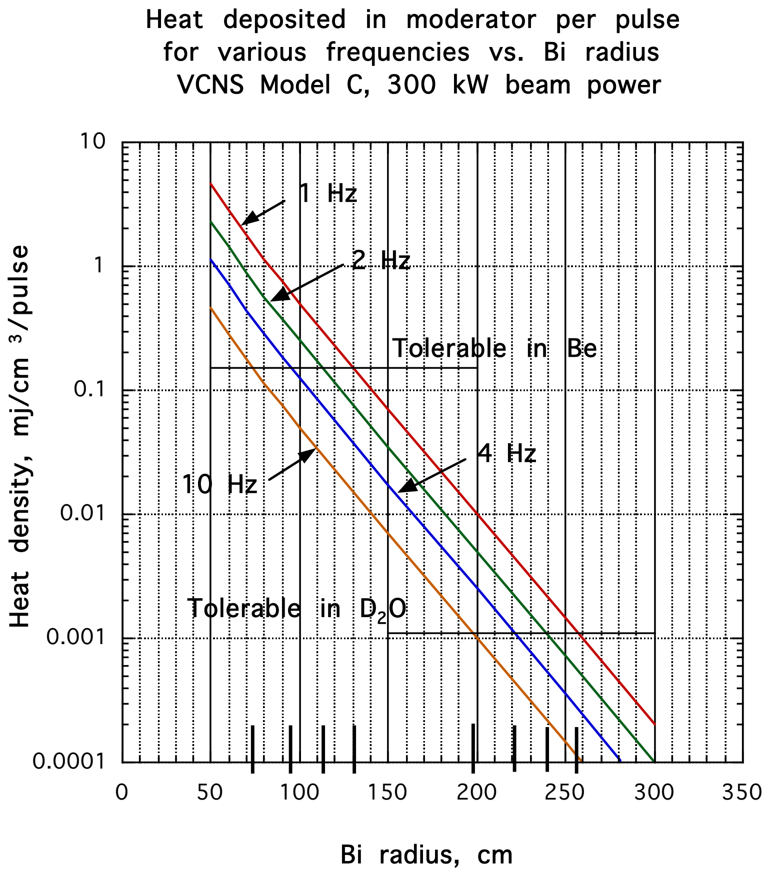
VCNS Monte Carlo Results
first round



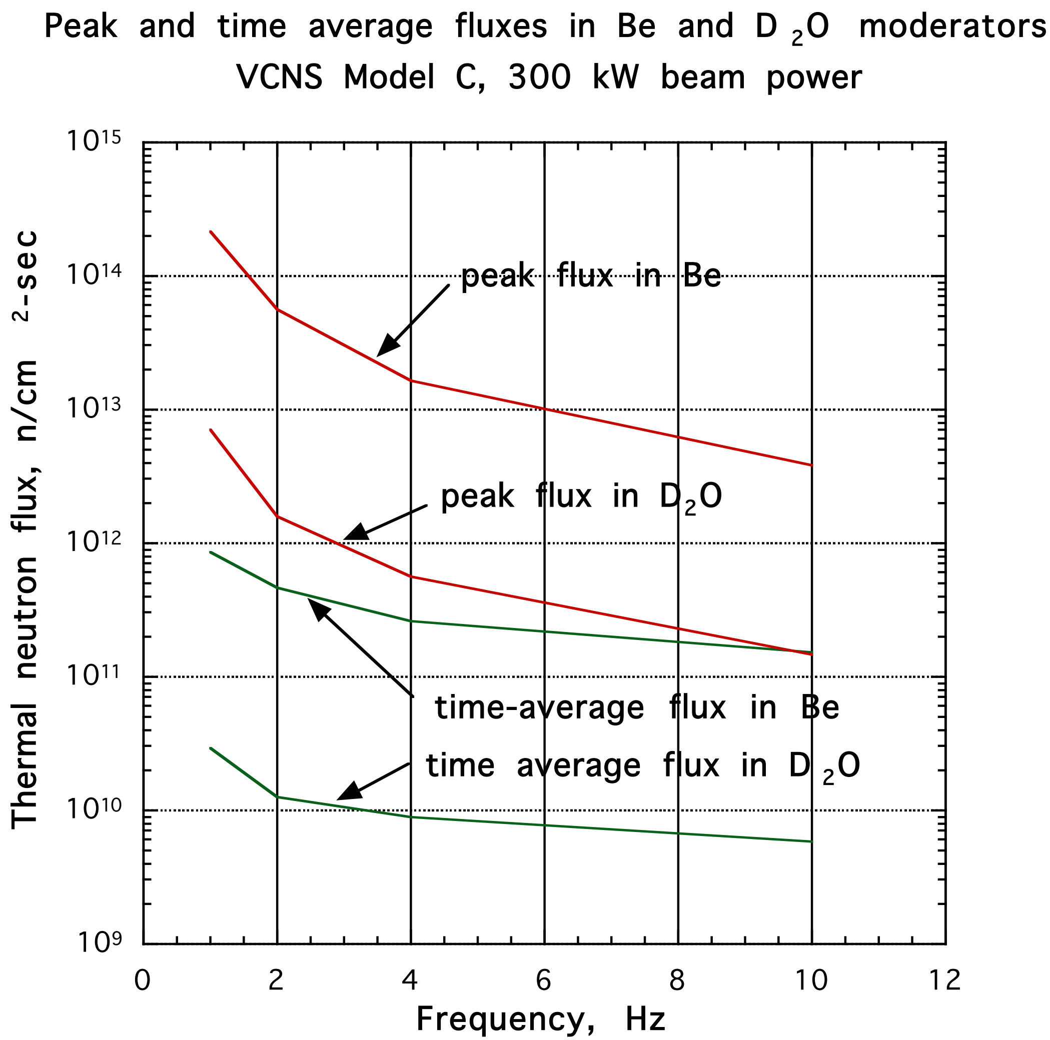


VCNS Monte Carlo Results





VCNS Monte Carlo Results

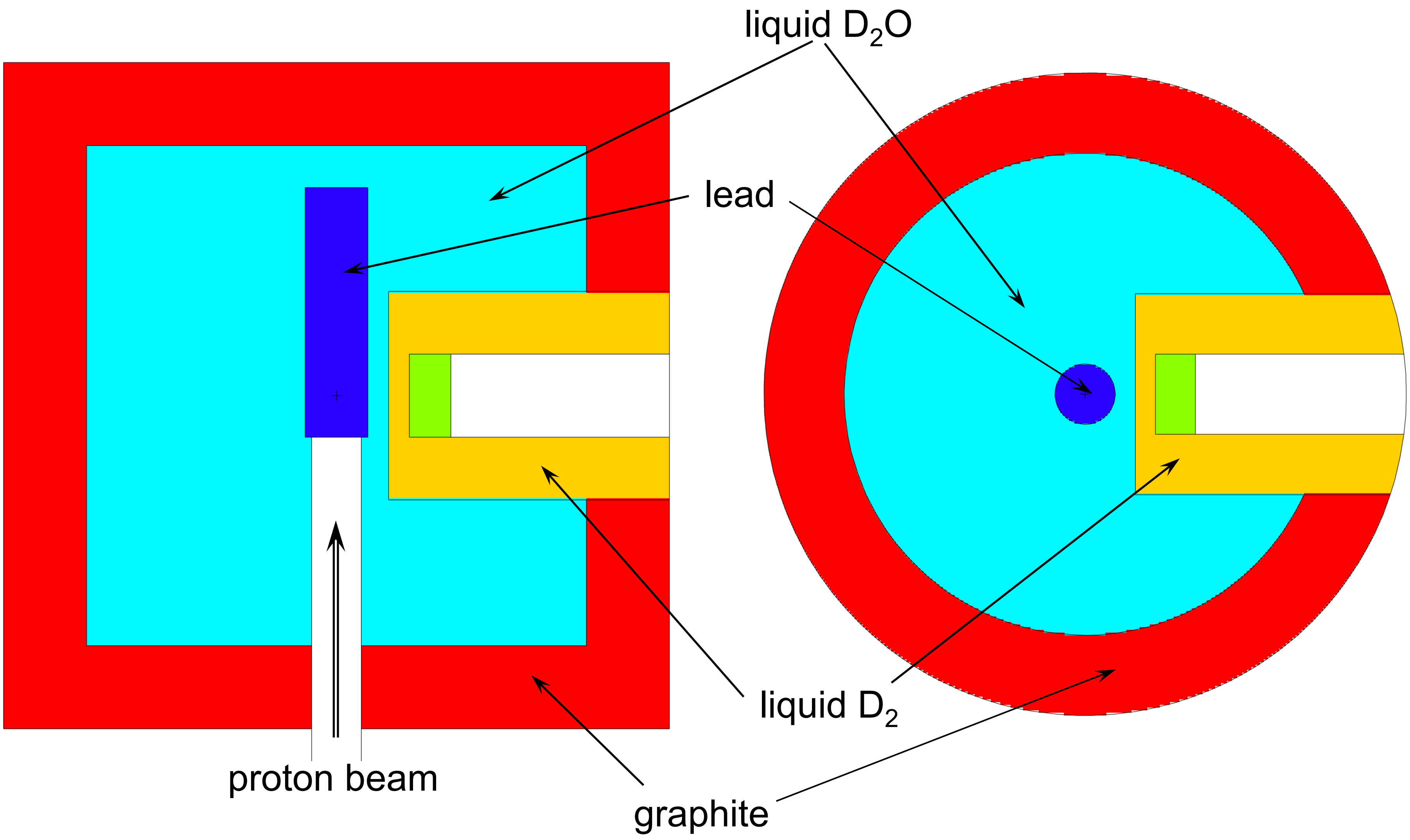


What Does a VCN/UCN Source Look Like?

- Typical UCN source configuration includes
  - Warm moderator (D_2O, ~ room temperature)
    - Choice of warm moderator affects rise/fall time of neutron pulse
  - Cold moderator (liquid D_2, ~ 20 K)
    - Some results have indicated that an intermediate temperature moderator is not necessary
  - Ultra-cold moderator (0.2 – 5 K)

- Study general properties of VCN source in warm moderator
  - Thickness
  - Location with respect to target
  - Target parameters

Representative VCN Source Model



Design Constraints

- Target heating
  - What will the target be (plates, liquid metal)?
  - Can we cool the entrance window and the high-energy portion of the target?
  - This consideration places a maximum limit on current density ($\mu A/cm^2$) during a pulse
- Moderator heating
  - Total energy deposition in moderator
  - Peak energy deposition in space and time
  - Can the moderator be cooled enough to prevent an unacceptable rise in temperature during a pulse?
  - Heat capacity and thermal diffusivity of materials are critical
  - This consideration places a limit on energy deposition in moderator
- Together these will limit the available neutron flux

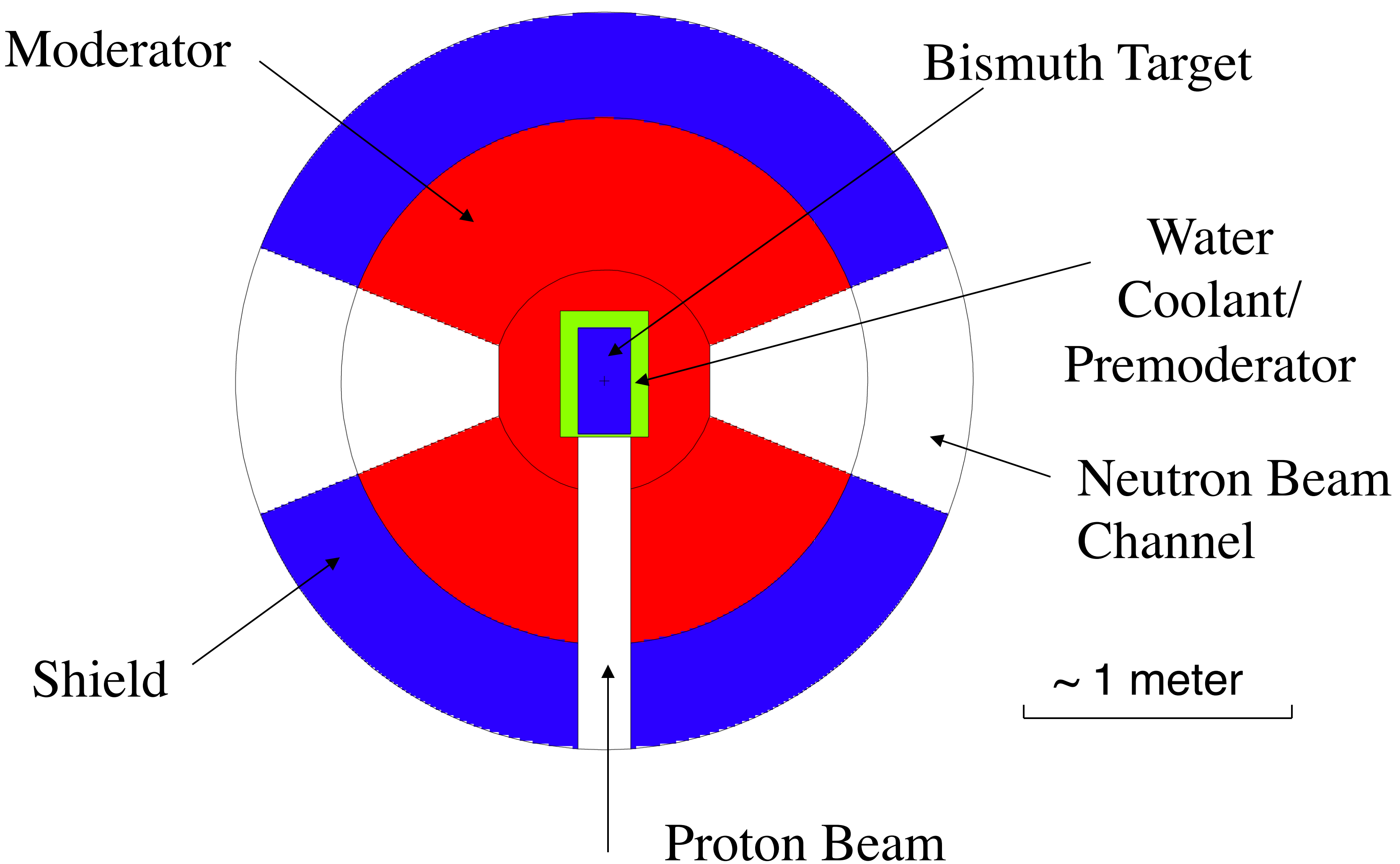
Requirements for Computation

- Code
  - MCNPX version 2.5.0
- Model
  - We use simplified geometric models
  - Both obvious and subtle effects will be left out
  - Real-world performance will be less
- Data
  - Good calculations require good data
  - Neutron scattering kernels do not yet exist for the materials, temperatures, and energies of interest
- How to proceed? We can either …
  - Perform simulations with free gas kernel (not ‘wrong’, just an approximation)
  - Calculate using known kernels and extrapolate from experiment

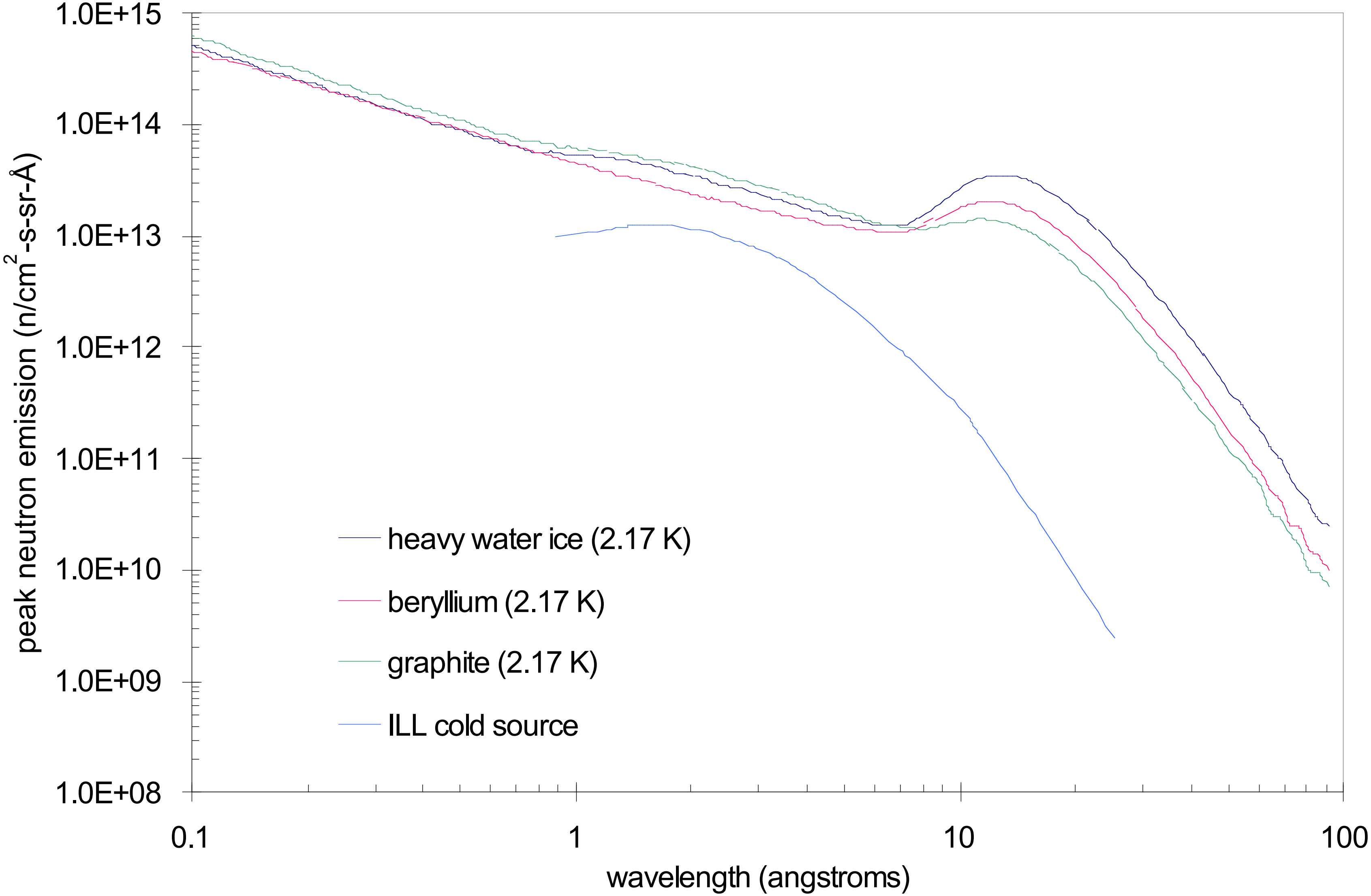
Preliminary Modeling

- Needed to get some idea of neutron emission spectra, intensities, and pulse widths
- These studies treated low-temperature scatterers as free gas
- Model highly generalized

MCNPX Model A

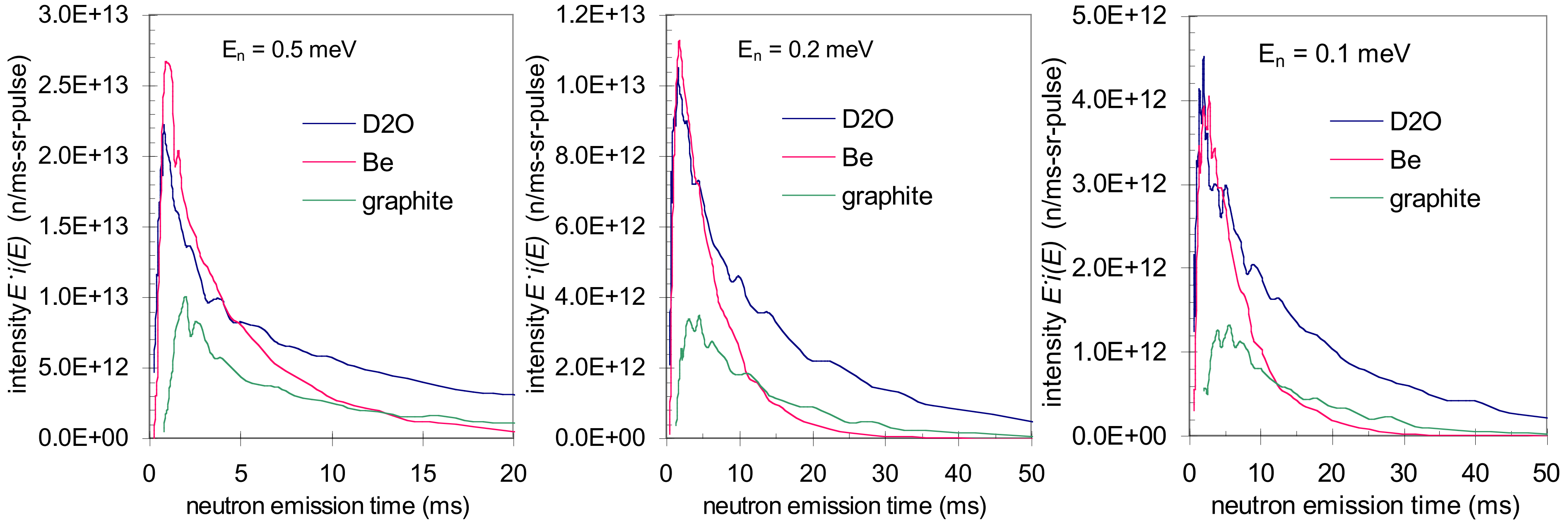


MCNPX Model A – Spectra



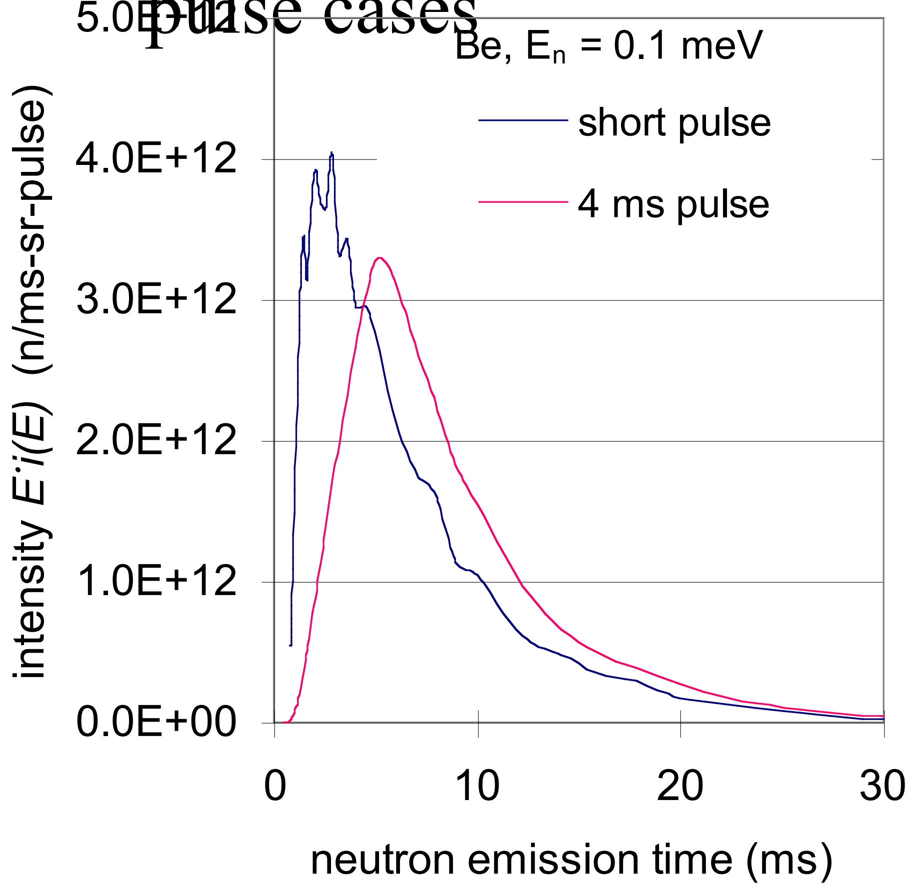
MCNPX Model A – Pulse Shapes

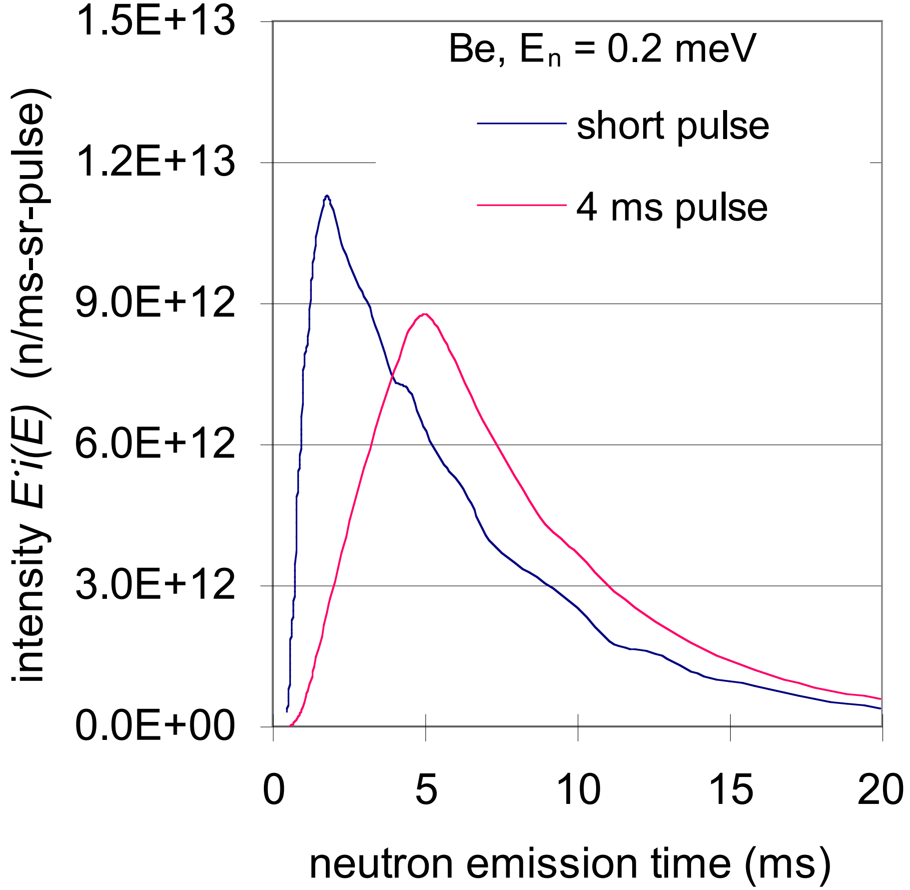
- Short-pulse time distributions



MCNPX Model A – Pulse Shapes

- Compare time distributions for short-pulse and 4-ms pulse cases





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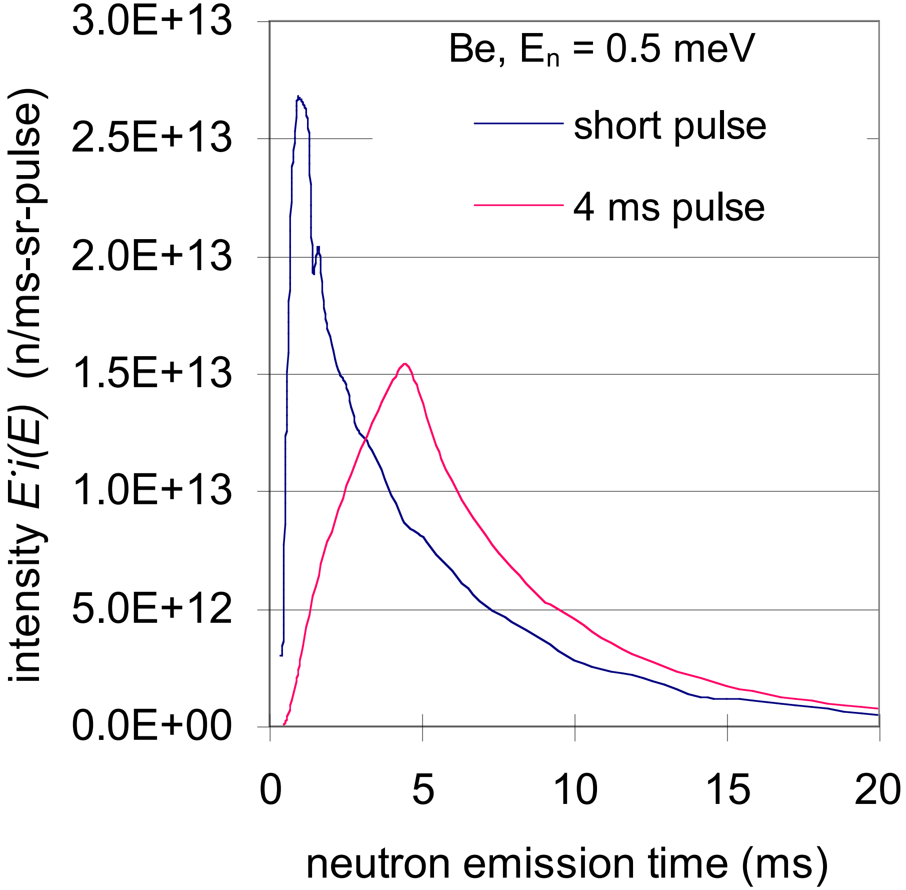
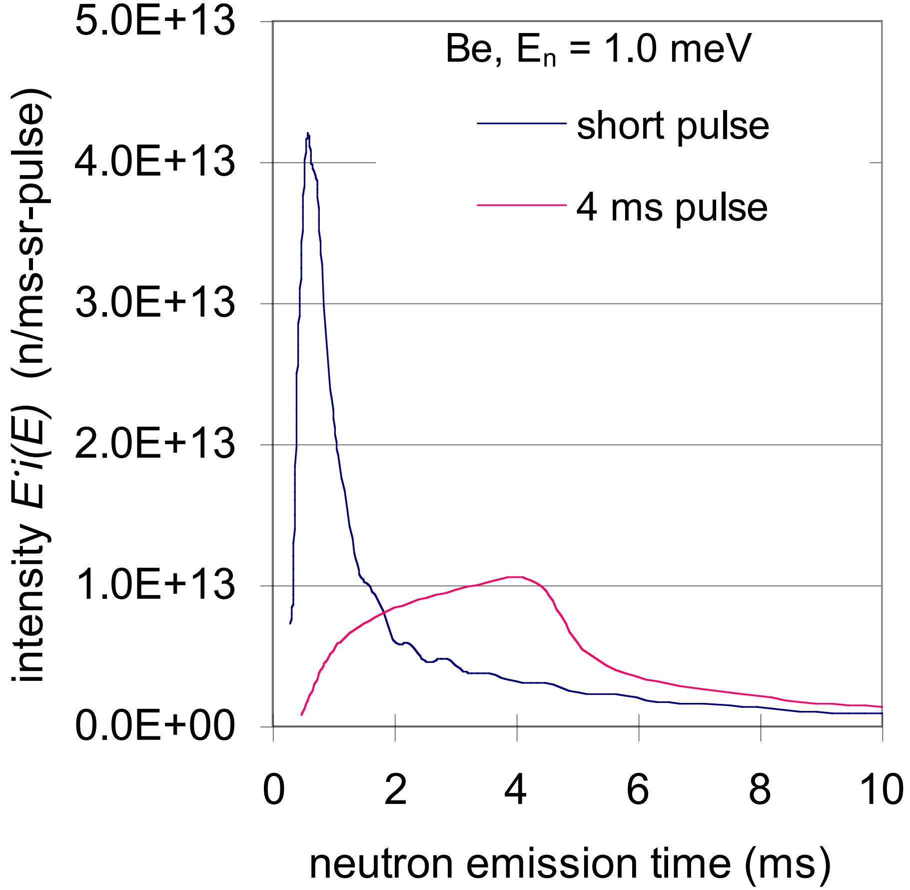


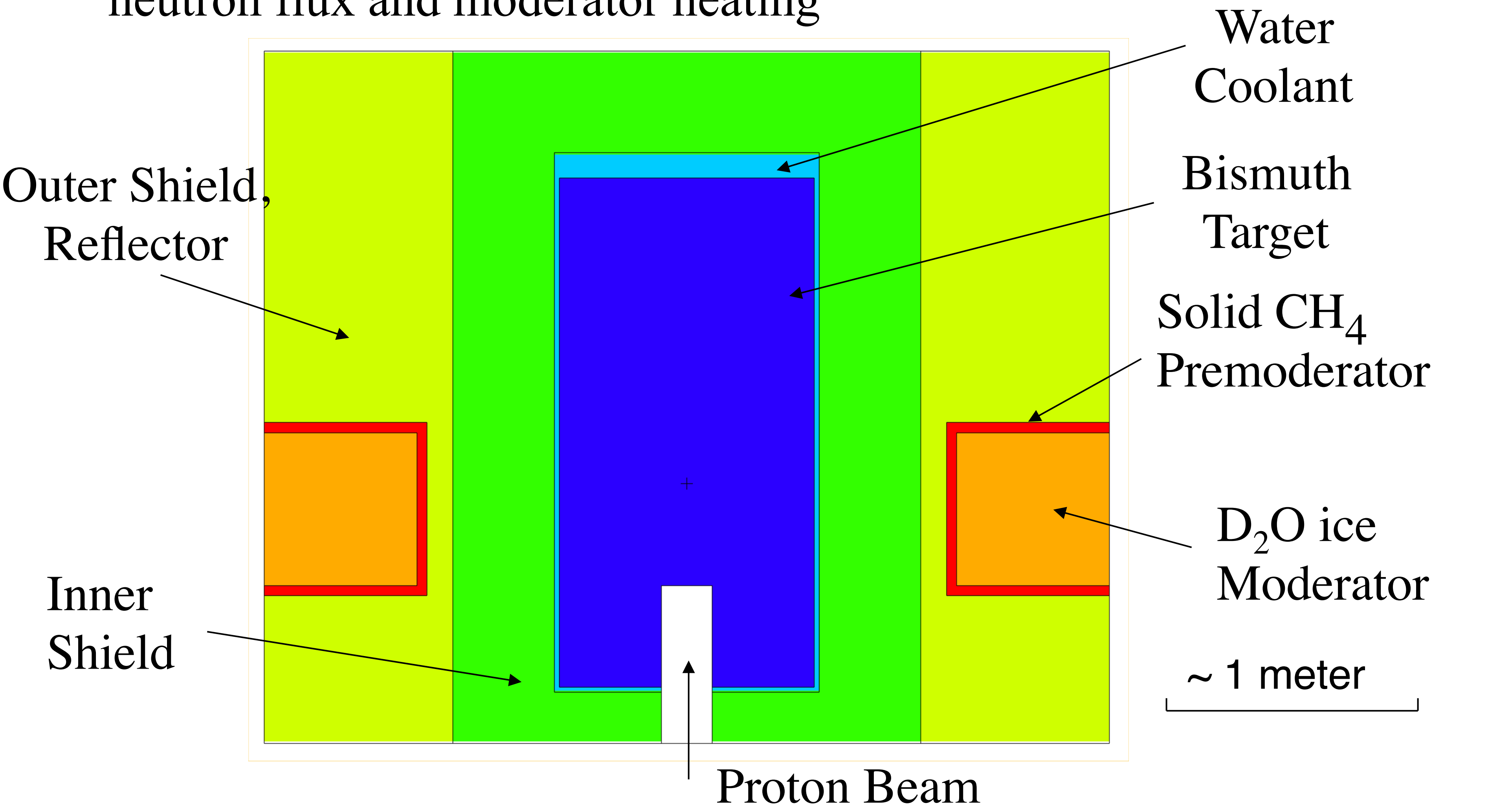


MCNPX Model A – Conclusions

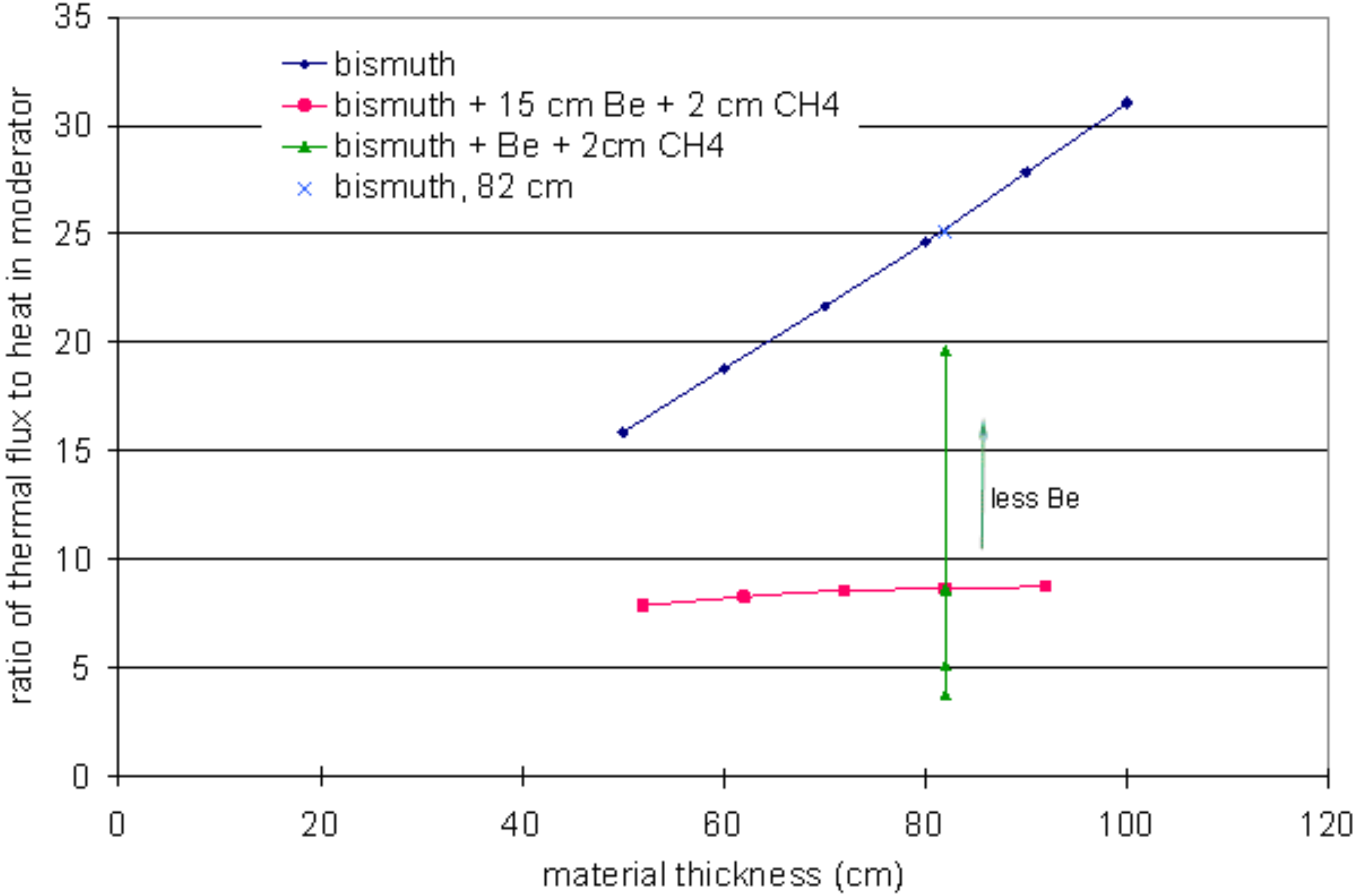
- Neutron pulse widths for the energies of primary interest are on the order of milliseconds
- Match the accelerator pulse length to this time scale
- 4 ms is longer than the typical ~ 1 ms traditional for a LPSS

MCNPX Model B (Cylindrically Symmetric)

- This model was used to study relationship between very-cold neutron flux and moderator heating



VCNS MCNPX Model B – Results



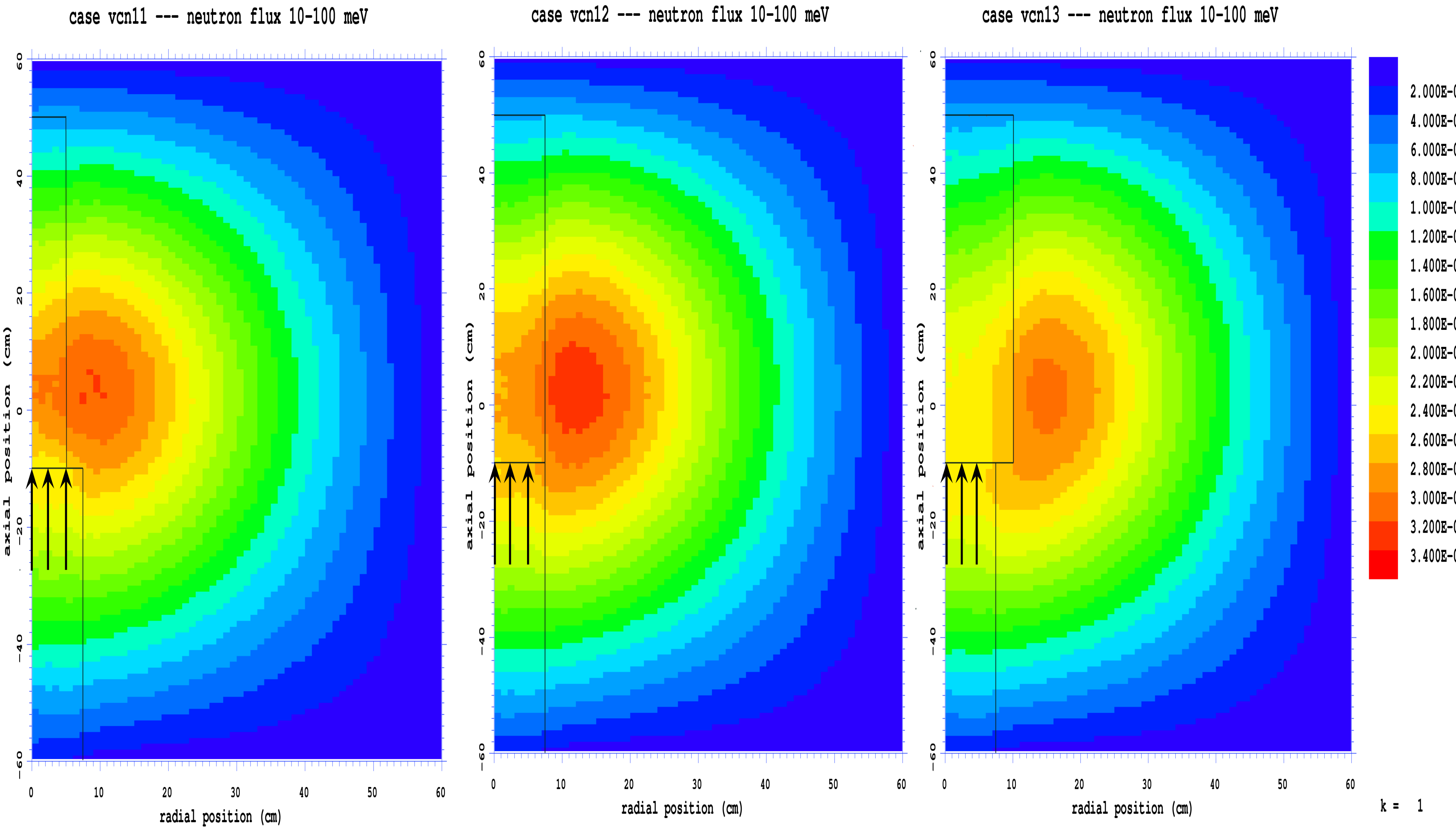
MCNPX Model B – Conclusions

- Metric of cold neutron flux per unit of energy deposited in cold moderator continues to improve as we move away from target, but at a cost in flux, to be made up by accelerator power.
- Heavy water a much better attenuator than bismuth – would a combination be better?
- Must avoid gamma generation near the cold moderator

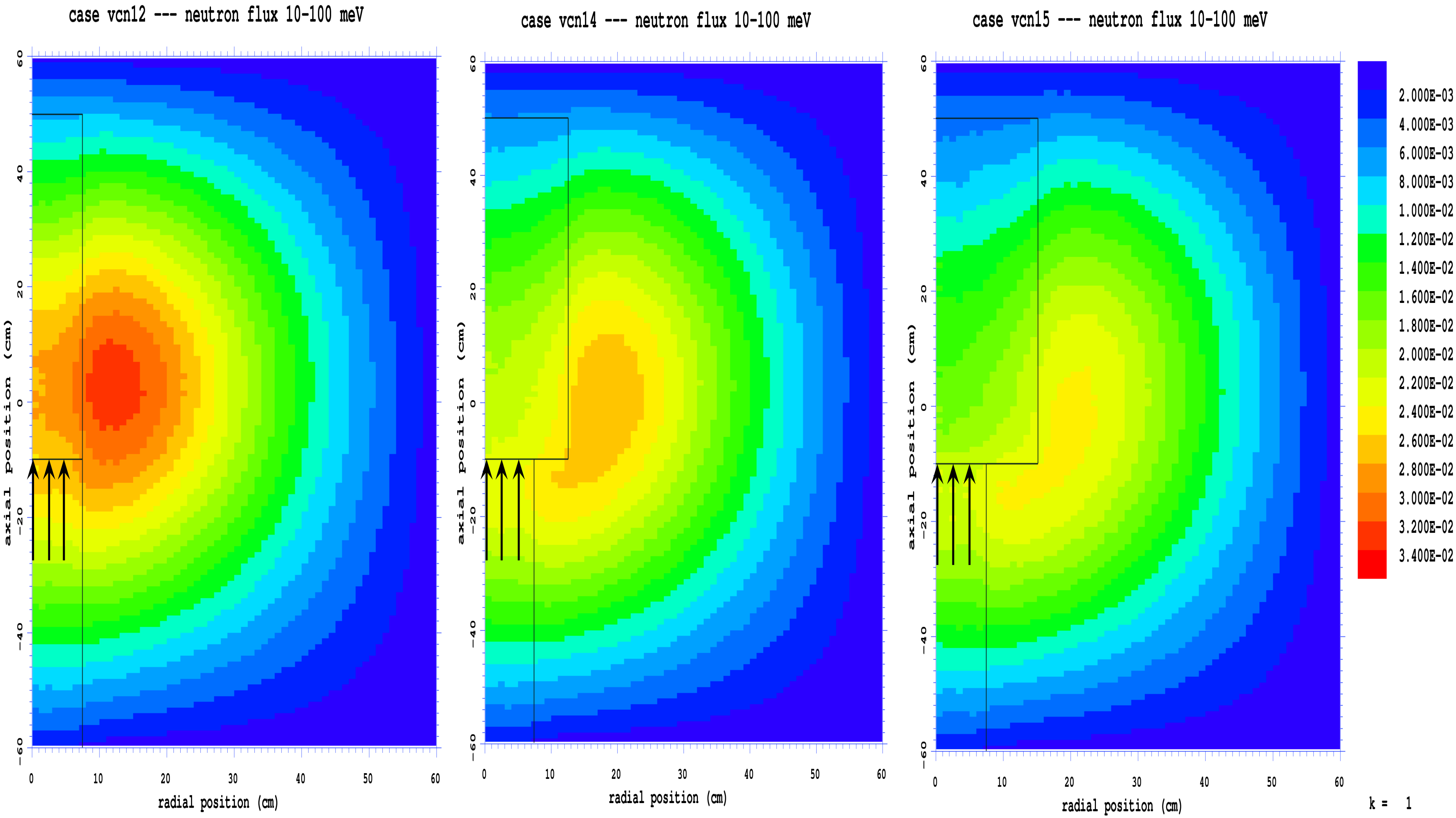
MCNPX Calculations for Warm Moderator

- Calculate flux profiles for selected combinations of beam and target diameter
- Two sets of calculations
  - First set – various sizes of target for constant beam diameter
  - Second set – using results from first set, keep R_{target}-R_{beam} constant and vary beam and target radii
- Examine results to find location of highest thermal neutron flux – this is where to put the cold moderator
- Use MCNPX mesh tally feature
- Profiles also give information on sensitivity of performance to exact position

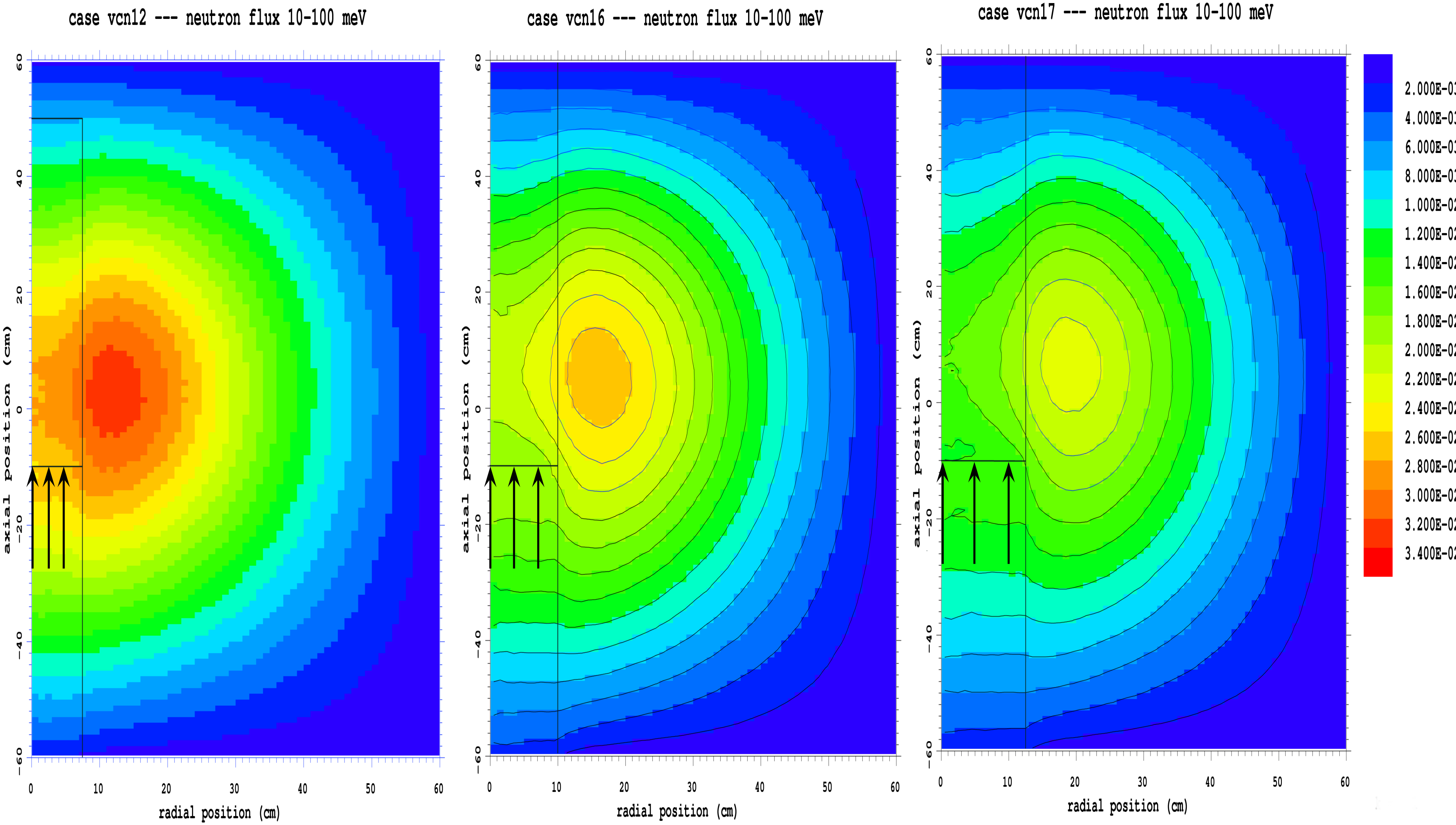
Neutron Flux vs. R_{target} (R_{beam} constant)



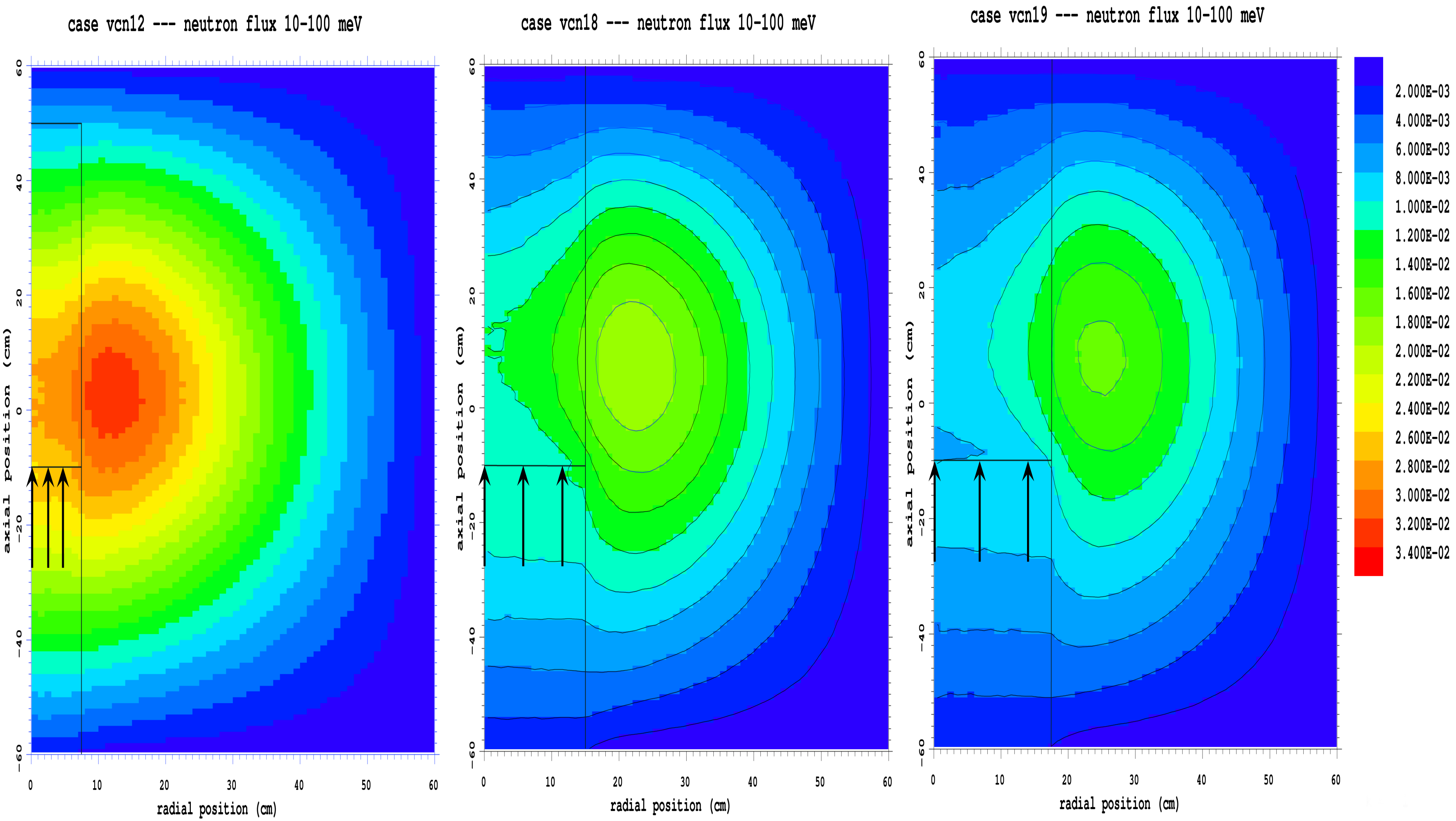
Neutron Flux vs. R_{target} (R_{beam} constant)



Neutron Flux (R_{target}-R_{beam} = 2.5 cm)



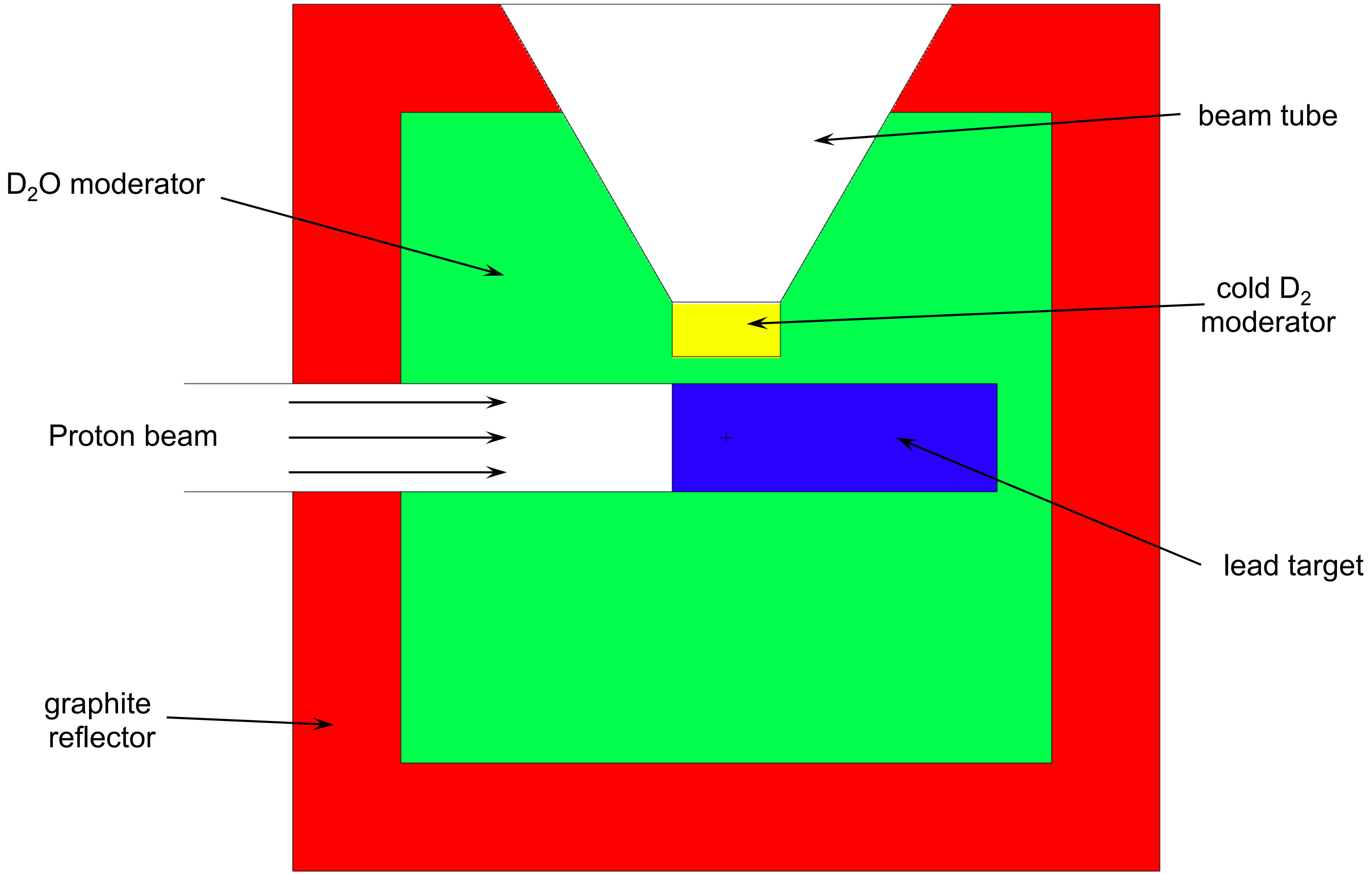
Neutron Flux (R_{target}-R_{beam} = 2.5 cm)



MCNPX Calculations for Cold Moderator

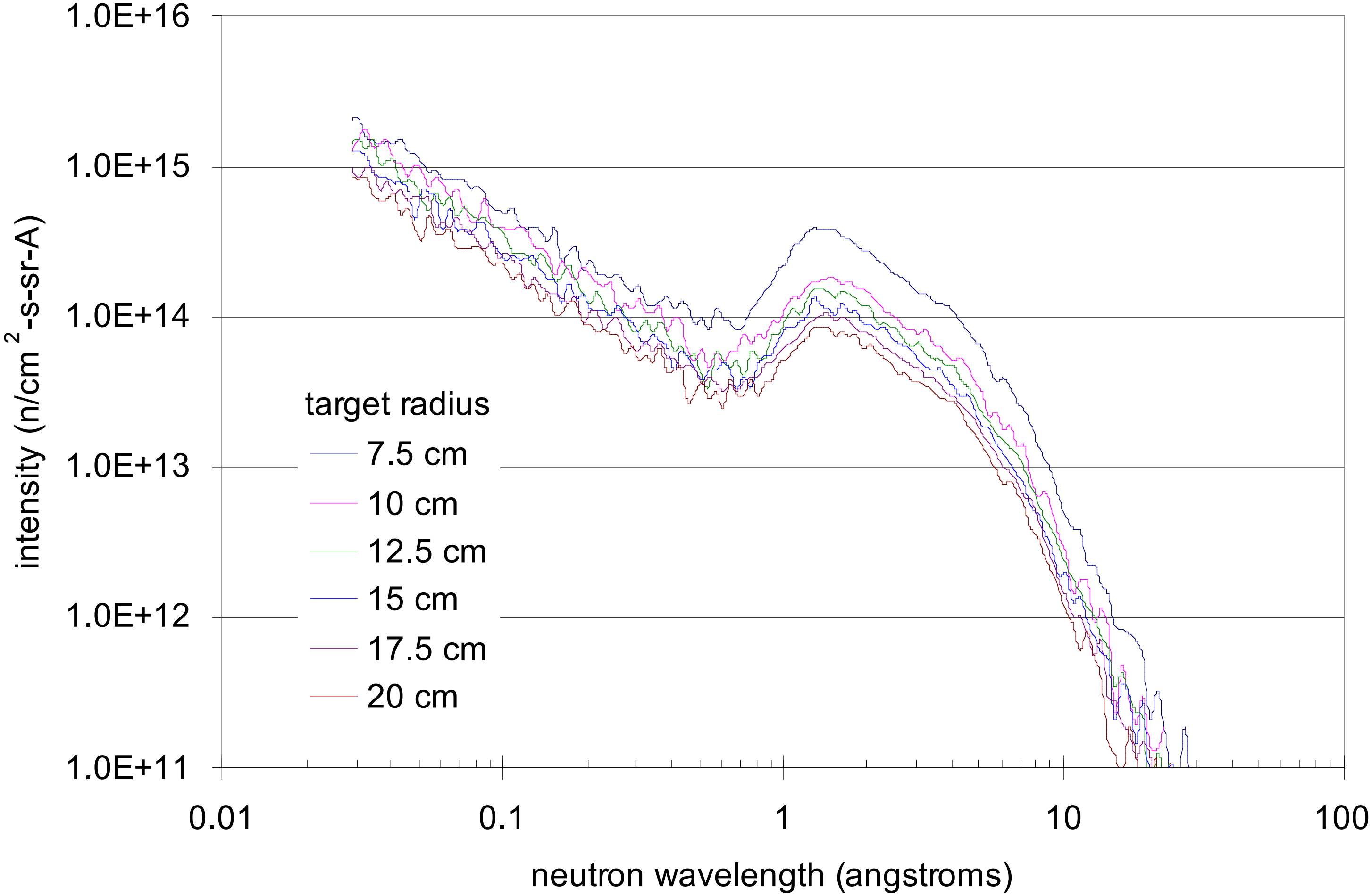
- Calculate neutron emission energy spectrum from surface of cold moderator
- Two sets of calculations
  - First set – fix position of cold moderator relative to target – keep R_{target}-R_{beam} constant and vary beam and target radii
  - Second set – for a given size of beam and target, vary moderator position (move further away)
- Examine results to find location where cold neutron flux is highest
- Look at results relative to peak volumetric energy deposition and total energy deposited in cold moderator
- Profiles also give information on sensitivity of performance to exact position

MCNPX Model for Cold Moderator



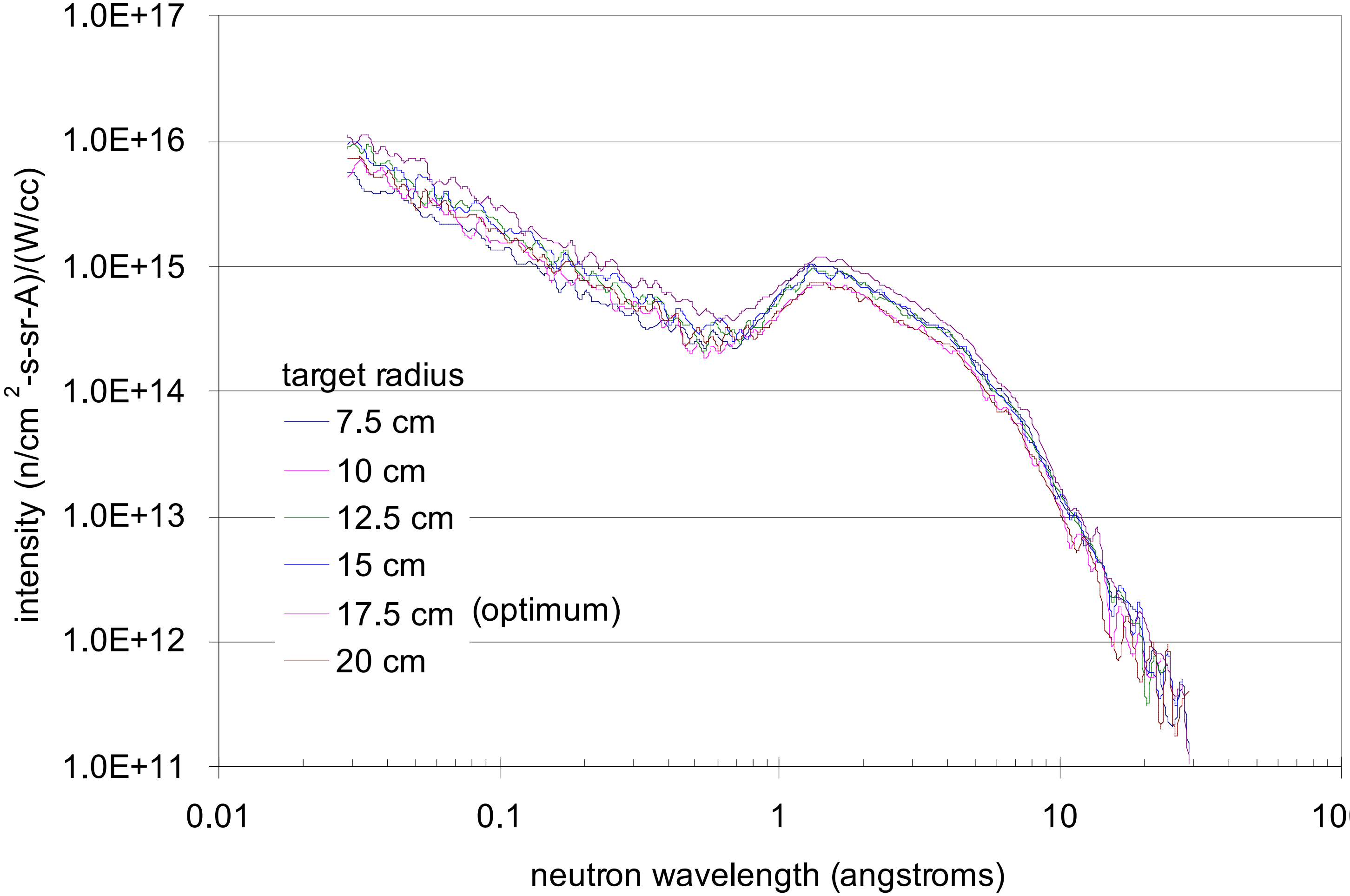
Neutron Flux vs. Target Radius

- Target and beam radii change together with R_{target}-R_{beam} = 2.5 cm
- The figure shows absolute neutron intensity



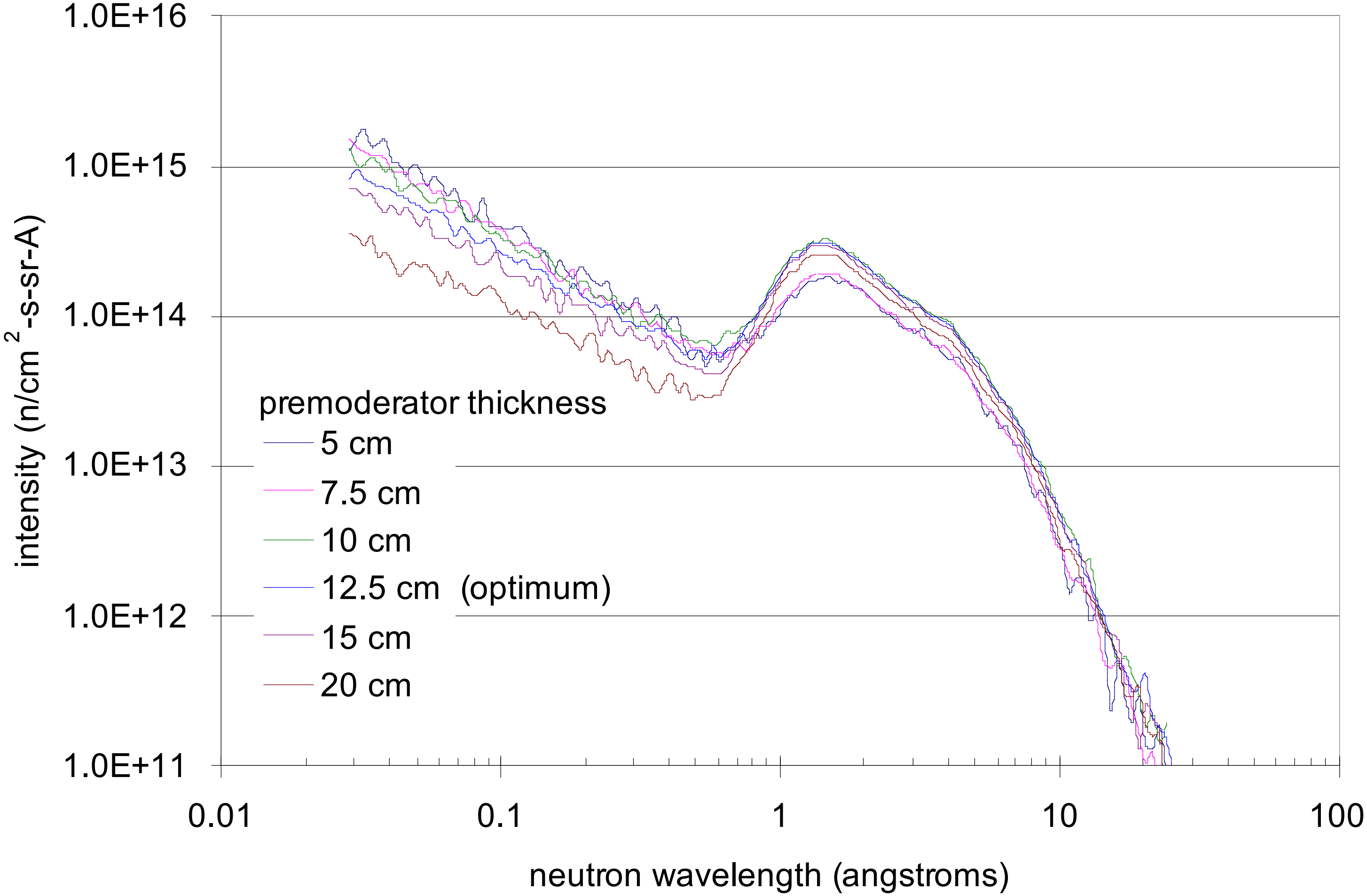
Neutron Flux vs. Target Radius

- Target and beam radii change together with R_{target}-R_{beam} = 2.5 cm
- Neutron intensity normalized to peak energy deposition



Neutron Flux vs. Premoderator Thickness

- $R_{target} = 10$ cm, $R_{beam} = 7.5$ cm
- The figure shows absolute neutron intensity



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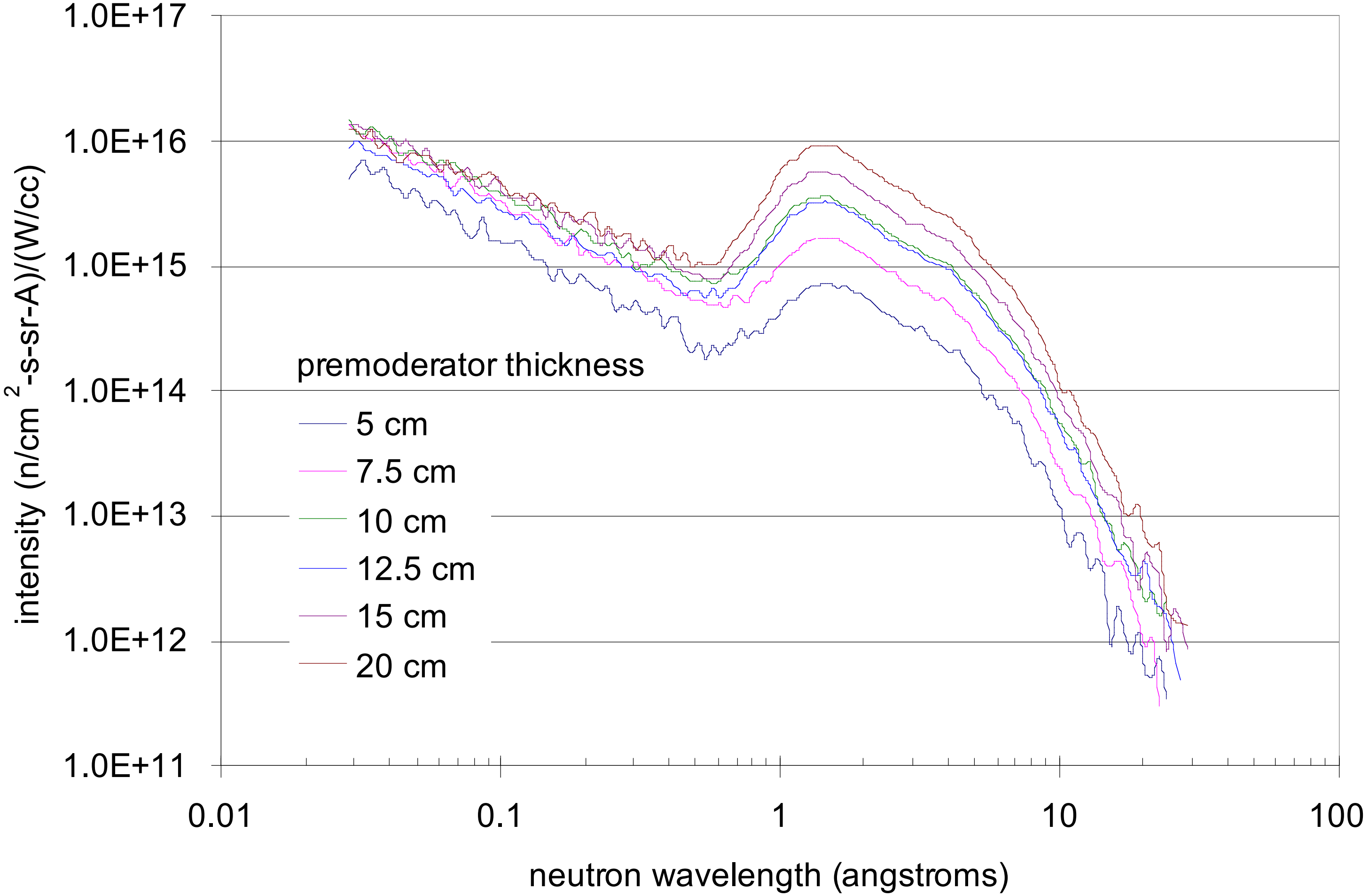
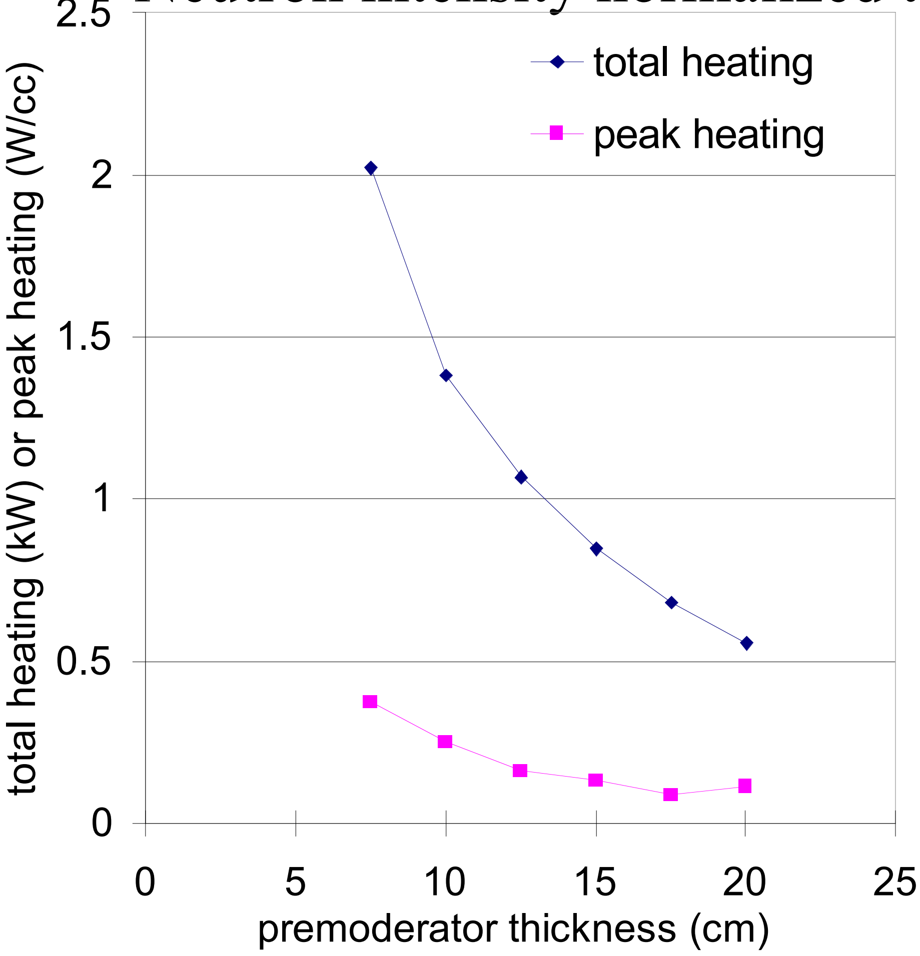
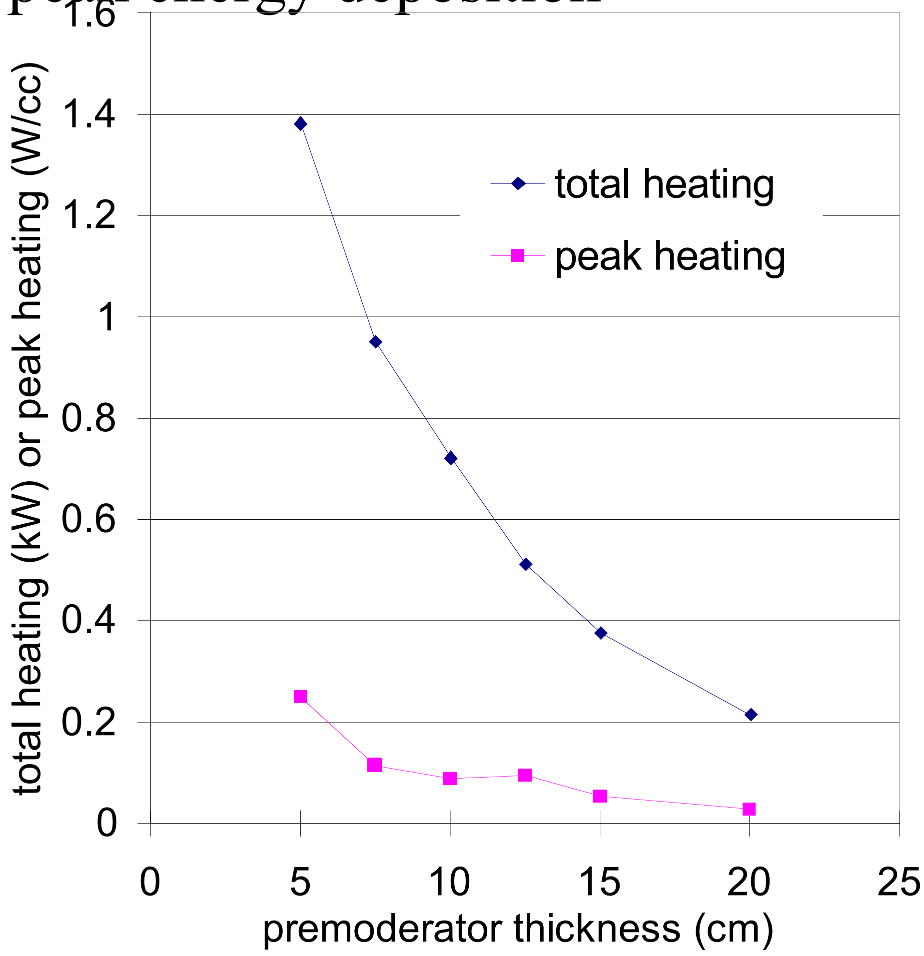


Cold Moderator Heating Results

- R_{target} = 10 cm, R_{beam} = 7.5 cm
- Neutron intensity normalized to peak energy deposition



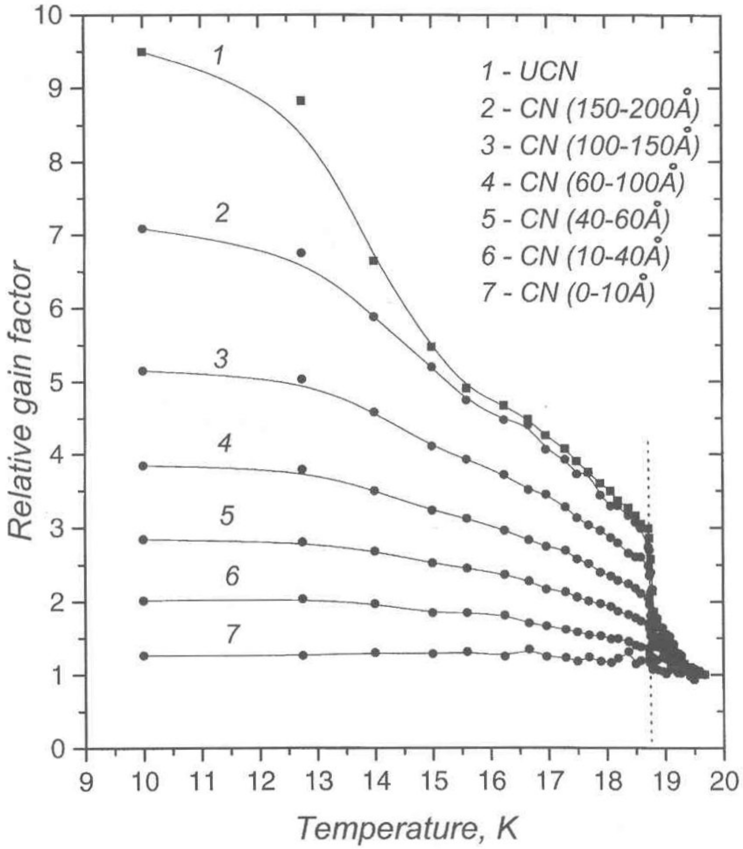


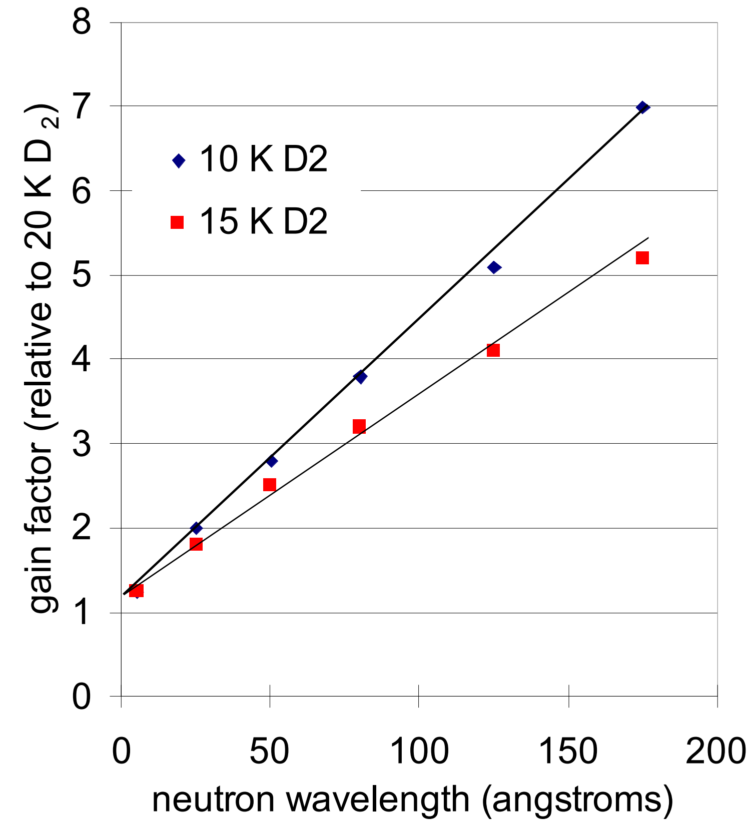
Scaling to Experimental Data

- There are experimental data on the gain in long-wavelength neutron flux as a function of moderator temperature in certain configurations
- We used these measured data to predict neutron flux for a 10 K D_2 or D_2O moderator based on simulations for a 20 K D_2 moderator
- Compute enhancement as function of wavelength
- We expect VCNS enhancement to be greater and extend to longer wavelengths, since the moderator volume will be significantly larger

Neutron Flux Scaling – D_2 moderator

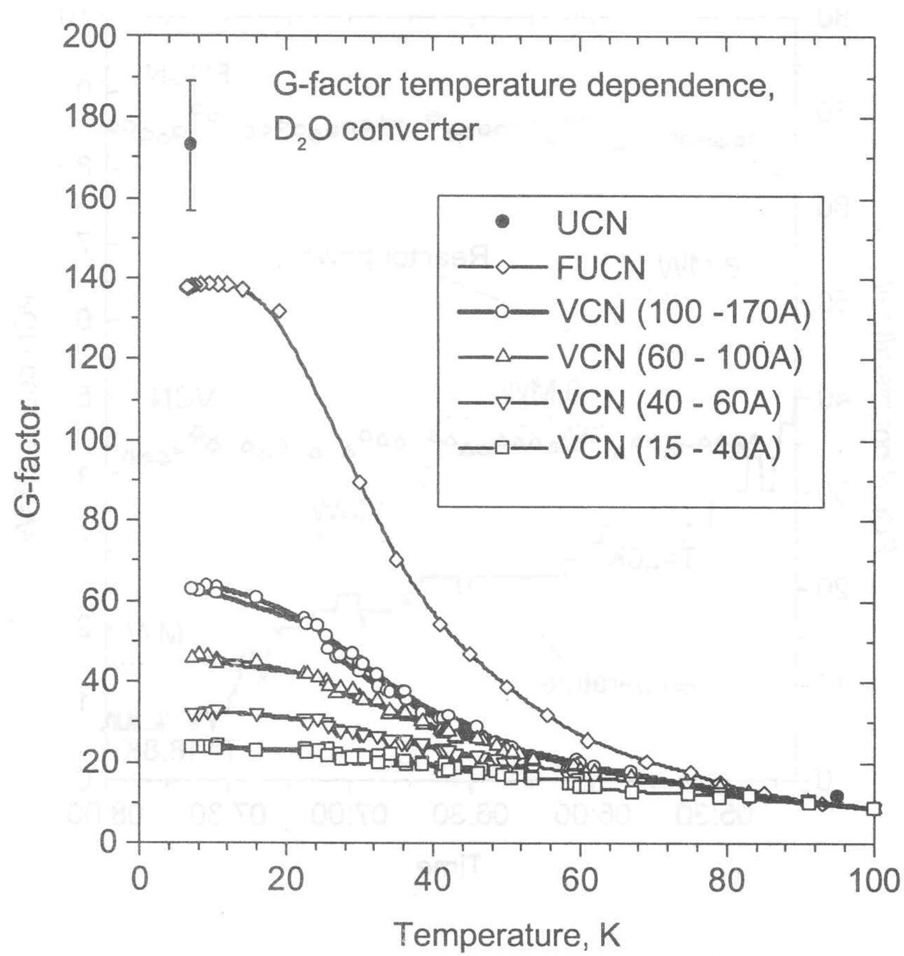
- Serebrov et al. measured flux gain factors relative to D_2 at 20 K
- Gain factor linear with wavelength, slope temperature dependent
- Larger gain extending to lower temperatures for larger system?



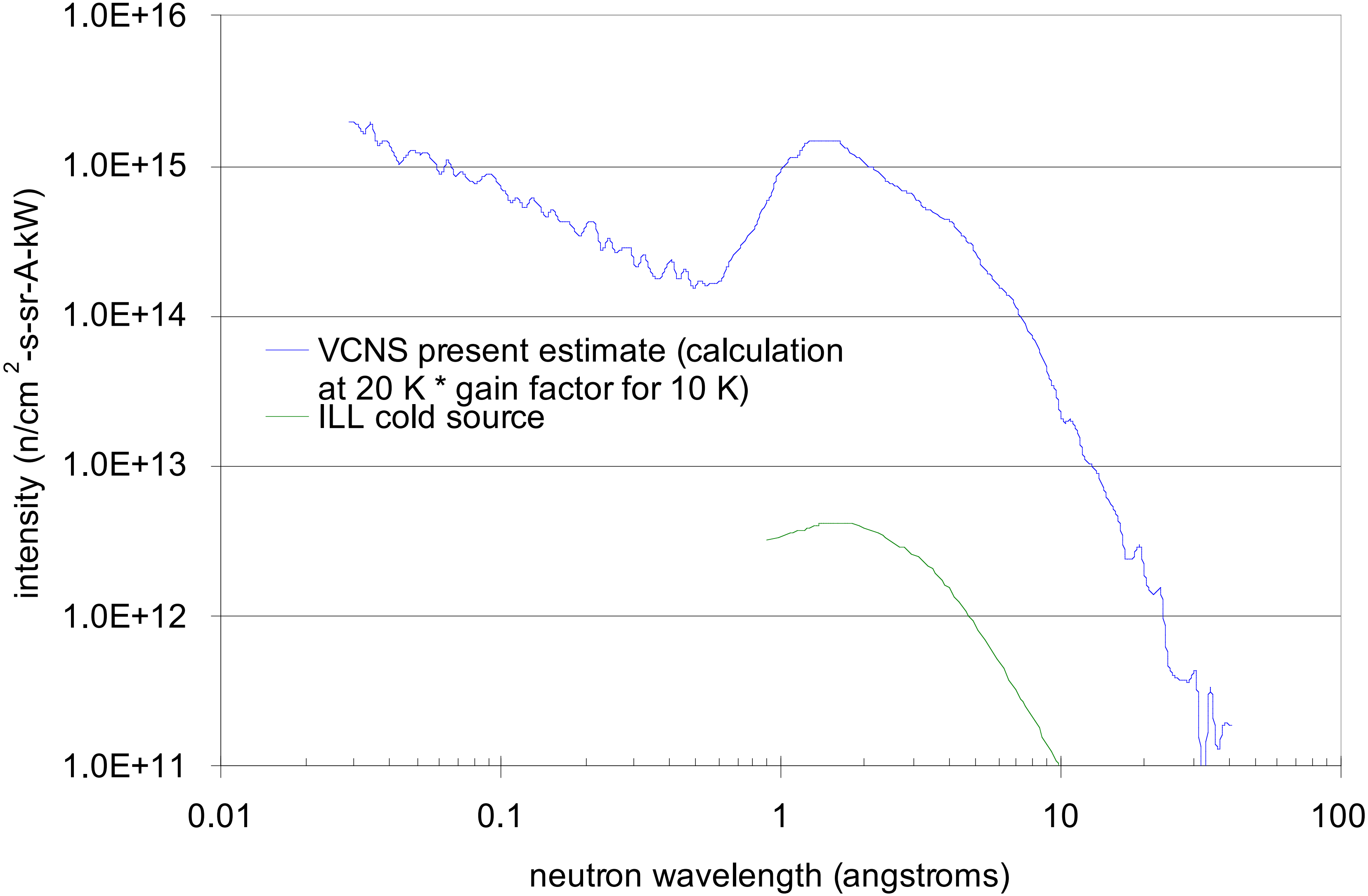


Neutron Flux Scaling – D_2O moderator

- Serebrov et al. also measured flux gain factors in D_2O relative to D_2O at 273 K
- Little if any gain as temperature is decreased below 20 K



Scaled Neutron Flux for VCNS Concept



Summary and Conclusions

- Scientific prospects for a VCNS are exciting!
- Much of the interest depends on the neutronic performance of the facility
- We do not presently have all the tools required to calculate source performance – in particular, the neutron scattering kernels for many candidate moderator materials do not exist for the temperatures and energies of interest
- We are working actively to address this problem
- Nevertheless, we have obtained some interesting and important results regarding VCN source design, and will continue our efforts

VCNS Workshop at Argonne

- A workshop to explore the interest from the scientific community in a VCNS was held at Argonne on 21-24 August 2005
- 39 workshop participants came from 12 US and international institutions
- Primary focus was to gauge interest in scientific applications of a facility delivering 30-1000 times the presently envisioned flux at 20 Å
- Participants received briefing materials beforehand
- Selected individuals gave prepared talks
- Participants came prepared to discuss the applications of the proposed facility
- Discussion groups formed in the areas of scientific applications, instruments & techniques, and sources

VCNS Workshop Participants

Jyotsana Lal
Peter Geltenbort
Marcus Blueul
Brad Micklich
Yasuhiro Masuda
Roland Gähler (*)
Manfred Daum (*)
Geza Zsigmond
Jim Richardson

Nicole Green
Erik Iverson
Michael Agamalian
Chen-Yu Liu
Sasha Kolesnikov
Jack Carpenter
Ferei Mezei
Steve Bennington
Stefan Rosenkranz

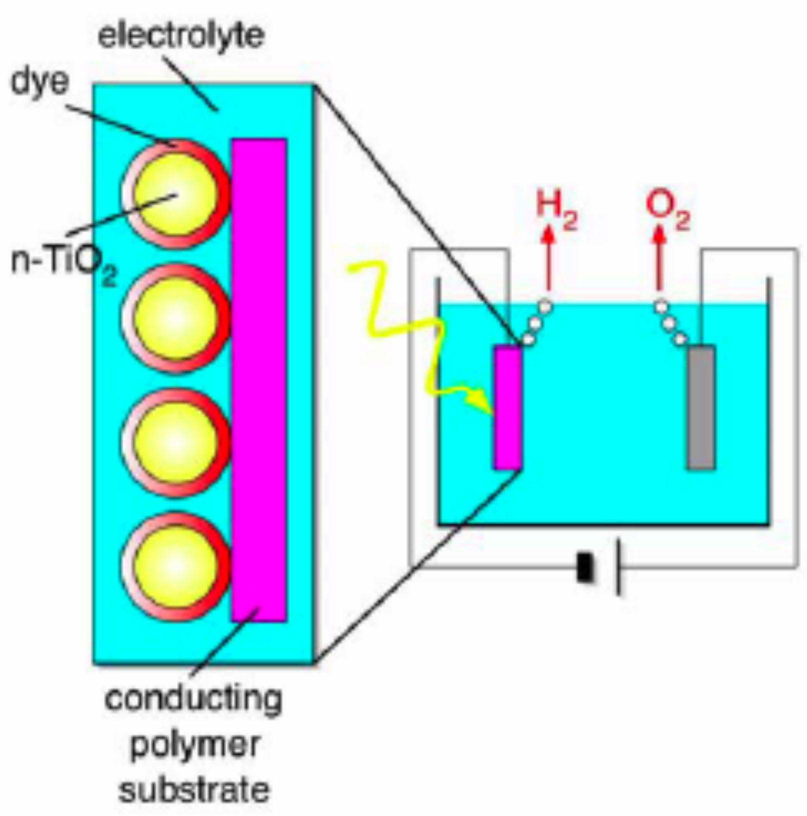
Gian Felcher
Yoshihisa Iwashita
Ken Littrell
Roger Pynn
Chris Benmore
Paul Sokol
Jim Rhyne
Art Schultz
Kent Crawford

Colin Carlile (*)
Hirohiko Shimizu
Gene Ice
Paul Brod
David Price
David Mildner
Masatoshi Arai
Chuck Majkrzak

(*) discussion group leader ANL USA Europe Asia

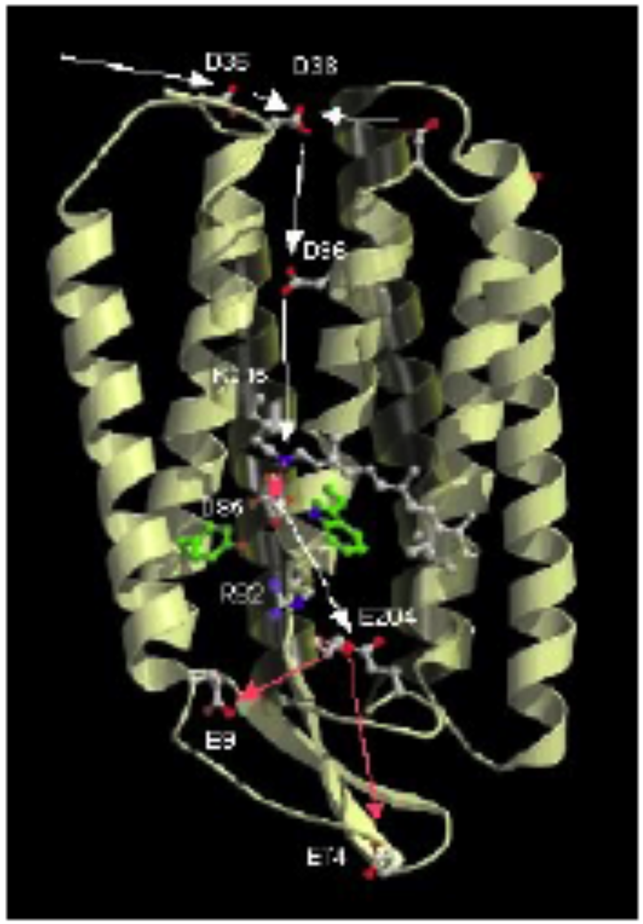
VCNS Applications

nanoscale-enhanced photocleavage of water



VCNS Applications

light-driven protein-based proton pump



VCNS Workshop – Major Conclusions

- There was a lot of excitement generated about the possibility of a VCNS, and the new types of science that could be possible
- Science working group
  - A VCNS would enable entirely new fields of research, and can greatly improve existing fields
  - Major advances are foreseen in the fields of
    - nanomaterials
    - soft matter dynamics
    - material contrast
    - microscopy / holography
    - spintronics
    - fundamental physics
    - energy & environmental technology
    - medical applications

VCNS Workshop – Major Conclusions

- Instrumentation working group
  - Properties of long-wavelength neutrons can be exploited to design novel instruments
  - Longer-wavelength spectrum improves other instruments
  - Beam modulation and spin echo methods look especially promising

- Source working group
  - Accelerator issues are well in hand
  - Primary outstanding issues are the need for neutron scattering data and technology for cooling the cryogenic moderator

- The workshop proceedings was published in March 2006.

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. We envision a second workshop.
- 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.