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Moderator Materials and Neutronic Performance

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The great variety of instruments proposed for LANSCE-II entails an equally varied set of requirements for the target stations moderators. Besides the obvious features such as intensity and pulse width of the neutron pulse, a number of more pragmatic questions have to be addressed such as fast neutron background and energy deposition in the moderators, especially at large proton beam powers such as the 1 MW proton beam power proposed for LANSCE-II.

Introduction

The moderator is the interface between the neutron production target and the instruments. It affects directly the performance of the instrument connected to it, and its optimization (materials, size, position, coupling/decoupling, poisoning, temperature, etc...) is therefore a most crucial aspect of target station design.

We review briefly the performance of light water, liquid methane, and liquid hydrogen moderators in flux-trap geometry. Various figures of merit such as peak intensity, integrated intensity, pulse width, pulse decay times, etc ... are tabulated systematically. These results were meant to serve as references for future studies.

The instruments proposed for the 1 MW sources at LANSCE and IPNS, and for the 5 MW source at the ESS will place further demands on moderators and moderators design that in some cases will require to go beyond the capabilities of the three traditional moderators mentioned above. To meet this challenge, we propose a new type of moderator, namely the composite moderator. The basic motivation behind the particular type of composite moderator presented below is spectrum mixing to produce neutron spectral characteristics that are well- or better-adpated to a given instrument. The results of computer simulations show that this particular concept seems to be very promising.

Another particularly important aspect of moderator research at pulsed spallation neutron sources is the moderator longevity. The intense radiation field to which a moderator is subjected, as well as the large amounts of energy deposited in the moderator conspire to compromise the mechanical integrity of the moderator assembly. This is the main reason that, so far, only liquid moderators have been used in practice at pulsed spallation neutron sources. The liquids used traditionally, namely light water, liquid methane, or liquid hydrogen, represent a good compromise between excellent resistance to radiation damage (with the exception of liquid methane) and ease of cooling, and a reasonable hydrogen density. Solid metal hydrides typically have significantly higher hydrogen densities, and so could potentially increase dramatically the performance of moderators for the next generation of pulsed spallation neutron sources. On the other hand, simple hydrides such as ZrH_2, for instance, suffer from the problem that the density of low energy vibrational modes that matter most for neutron thermalization is low compared to liquids. Although this is somewhat of a disadvantage for moderation to thermal energies, the material could still act as a very efficient premoderator. Altogether, little work has been done on the possibility of using solid metal hydrides for neutron thermalization, with the exception perhaps of ZrH_2 and TiH_2. The latter was investigated as a premoderator in the early days of the WNR facility at LANL. In particular, calculation of neutron scattering kernels in metal hydrides are inexsistent, not to mention a lack of knowledge of resistance to radiation damage, or basic mechanical properties in all but a few metal hydrides. Because of the potential advantages shown by solid metal hydrides moderator, we plan to investigate solid moderators in great detail in the near future.

Although we do not address directly the radiation damage aspects of moderator design, we describe the results of a number of computer studies regarding energy deposition in the moderators at LANSCE. The results of these studies should prove useful in estimating the cooling capacity required for typical moderators, and should help in estimating the lifetime and failure modes of moderators at a pulsed spallation neutron source.

Reference moderators

Traditionally, three types of moderators have been used at spallation sources. Light water moderators produce a neutron spectrum peaking at about 40 to 50 meV; liquid methane moderators peak at about 10 to 20 meV and liquid hydrogen moderators spectra show a maximum around 2-3 meV. By suitably poisoning and decoupling these moderators, the pulse shape can be varied to meet different resolution or intensity criteria imposed by the instruments. We have examined in detail how these reference moderators would perform at a typical LANSCE-II spallation target, and paid attention not only to major features such as neutron beam intensity and time distributions, but also to arguably less crucial characteristics such as fast neutron background.

The first step in the moderators selection process is to assess the users' needs. In order to help the users in making this choice, we studied a number of reference moderators, and characterized them in detail:

- high-resolution H_2O; Gd poison
- high-intensity H_2O; Gd poison
- liquid H_2 (decoupled), no poison
- liquid H_2 (coupled), no poison
- H_2O/liquid H_2 (decoupled), no poison
- H_2O/liquid H_2 (coupled), no poison
- H_2O/Gd/liquid H_2 (decoupled), poisoned
- H_2O/Gd/liquid H_2 (coupled), poisoned

Moderator	Peak intensity (n/p/sr/μs)	FWHM (μs)	Rise time (10%-90%) (μs)	Decay time (μs)
H_2O high-intensity	0.00075	28	5	24.7
H_2O high-resolution	0.00071	16	4	11.7
Liquid CH_4, high-intensity	0.00088	20	4	34.0
Liquid CH_4, high-resolution	0.00087	13	4	20.2
H_2, decoupled	0.00083	22	6	83.7
H_2, coupled	0.00082	33	6	169.4
H_2O/H_2, decoupled	0.00076	23	6	113.0
H_2O/H_2, coupled	0.00076	33	6	217.1
$H_2O/Gd/H_2$, decoupled	0.00063	18	6	73.7
$H_2O/Gd/H_2$, coupled	0.00063	26	6	132.4
H_2 high resolution (boral)	0.00029	13	4	70.0

Table 1: Neutron pulse characteristics

- H_2 high resolution (decoupled with boral), no poison

The study was performed for these moderators in flux-trap geometry. The computer model for the target/moderator/reflector/shield assembly used in the simulations is shown in Fig.1.

In each case, we considered four identical moderators. The moderators were all 13 x 13 cm^2 moderators. The geometry was always kept fixed; we changed only the moderator material. For a LANSCE-II configuration with 2 flux traps, a reasonable rule of thumb is to decrease the flux by 20 % (relative to the one-flux trap geometry used in the present study) if the moderator belongs to the downstream flux trap, and 35% if the moderator belongs to the upstream flux trap. The moderator thickness is 4 cm for the H_2O moderators with the poison layer 2.5 cm from the viewed surface for high-intensity moderator, and 1.5 cm from the viewed surface for the high-resolution moderator. The liquid CH_4 moderators are 4 cm thick. The liquid H_2 moderators all have a 5 cm H_2 moderator. When the moderators are decoupled, the decoupler is usually Cd, 32 mils thick. The H_2O and liquid CH_4 moderators are always decoupled. The high-resolution liquid H_2 moderator is decoupled with boral. The calculated values for the liquid methane moderator are in very good agreement with the values measured by J. Carpenter et al. [1].

The studies illustrate the effects of coupling and poisoning moderators, and the effect of premoderators. The results cover a fairly broad range of neutron pulse characteristics, that are to be regarded as typical for LANSCE-II instruments design. Features such as pulse width in a given energy range, decay times in the time distributions, and peak intensity, for instance, were tabulated from Monte-Carlo simulation. In Table 1, the peak intensity, full width at half maximum, rise time (from 10% to 90% of the peak intensity), and decay times are given for all of the above moderators. All neutrons with energy less than 100 meV were included.

In the case of the water moderators, we also studied systematically the effect of varying the thickness of the premoderator while keeping the moderator thickness constant at 2.5 cm. The moderator was poisoned with 2 mils of Gd between the premoderator and the moderator. From the results shown in Fig.2, it can be seen that, up to a point, the useful

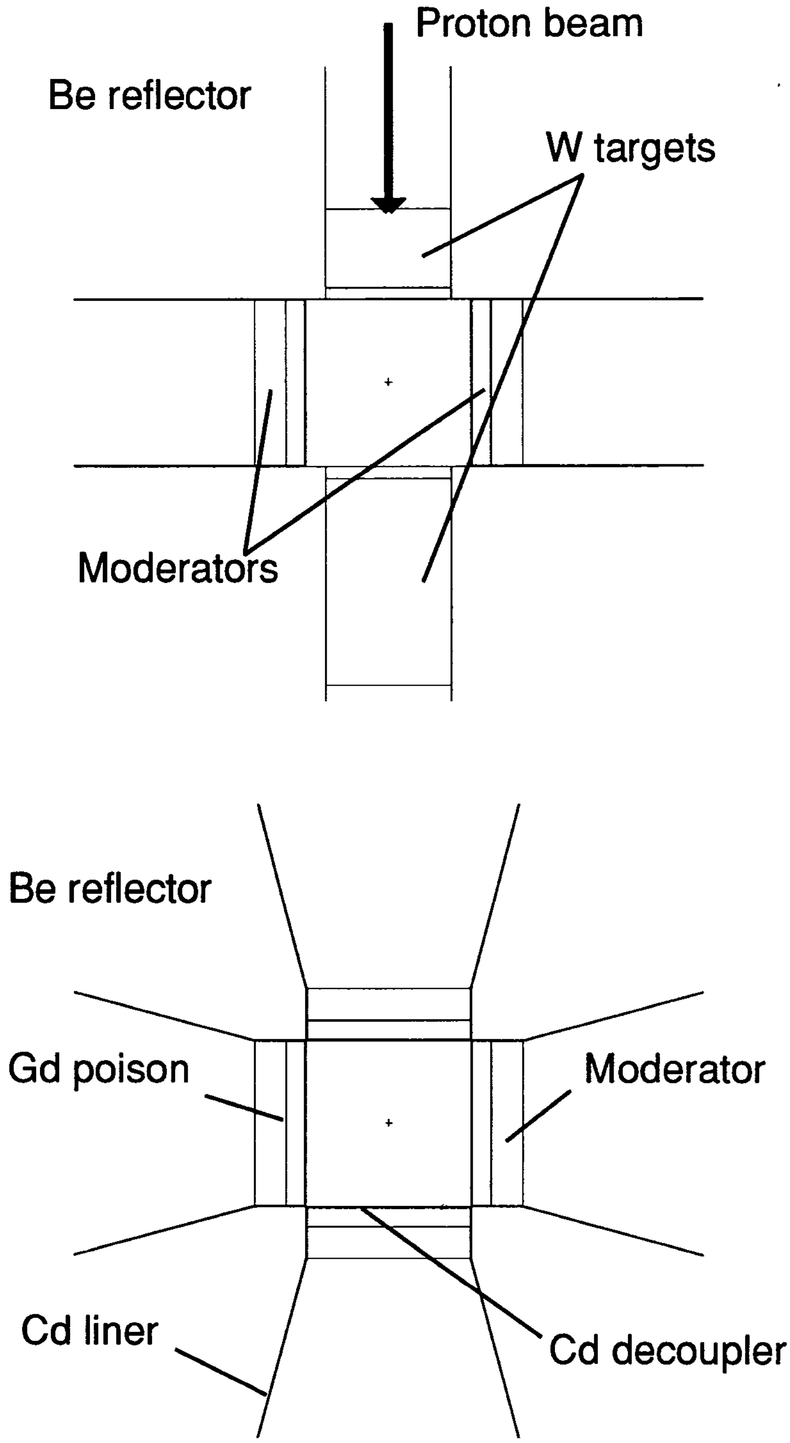


Figure 1: The simplified flux trap geometry used in the calculation of the reference moderators. The top figure is a vertical cross-section of the model; the bottom figure is a horizontal cross-section at the flux trap level.

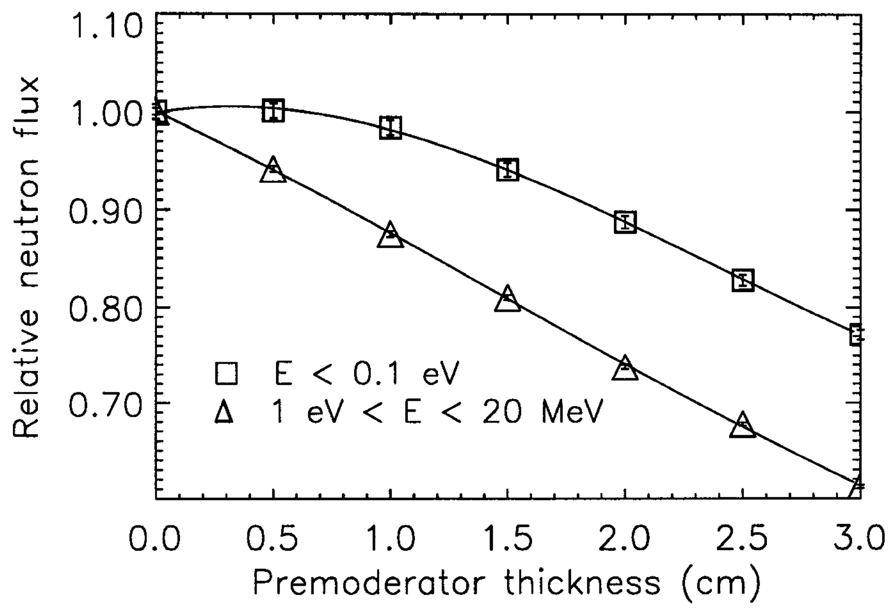


Figure 2: Effect of the premoderator thickness on the performance of a light water moderator in flux trap geometry

signal is unaffected, but the fast neutron background can be substantially reduced if the adequate premoderator thickness is selected. Although maybe not an issue at lower powers, this could become important at 1 MW. Notice that if the premoderator thickness is too large, the neutrons moderate exclusively in the premoderator and never get a chance to leak in the moderator through the Gd poison. This explains the decrease in useful signal intensity as the premoderator thickness is increased.

Composite moderators

In order to go beyond this traditional set of moderators, we propose a new moderator concept. For lack of a better term, these moderators will be refered to in what follows as composite moderators. A composite moderator is made of two (or perhaps more) layers of distinct materials. This by itself is not a new idea, and the concept of a premoderator/moderator assembly has been proposed previously: The premoderator material with a larger scattering cross section at higher energies scatters the neutrons down to a lower energy, and feeds them to the moderator layer where they are more rapidly and easily moderated to thermal energies [2-5]. The composite moderator (or what we call here a composite moderator) serves a different purpose. The idea is to mix the neutron spectra of two different materials to obtain an intense "broadband" neutron spectrum [5].

A good example consists in trying to emulate a methane spectrum by mixing a water spectrum with a liquid hydrogen spectrum. This is realized in practice by having a thick layer, say, a few cm, of water followed by a thin layer, say less than 1 cm, of liquid hydrogen. The viewed surface is the liquid hydrogen layer. In this way, it is possible to see through the hydrogen layer into the water moderator. For this reason, a more appropriate name for what we call a composite moderator would be a moderator/moderator assembly, as opposed to the premoderator/moderator assembly already mentioned. Fig.3 shows how the spectrum varies with the relative thicknesses of the water and hydrogen layers. In this particular study, the total thickness of the moderator is kept constant at 5 cm. A 1 cm layer of liquid hydrogen may not appear to be much moderator material, but it should be recalled that the neutrons fed to the hydrogen layer have already been heavily thermalized in the water moderator so that it does not take much hydrogen to lower their energy further. The time distribution of the pulse from a composite moderator is reasonably good, e.g., the full width at half-maximum of the neutron pulse (E $<$ 100 meV) is $\sim$ 25 μs. Although the pulse width and decay time are slightly larger than for a methane moderator, the difference is probably not significant for most applications.

This kind of moderating assembly (the composite moderator) works very differently from the traditional premoderator/thick-moderator assembly where the spectrum seen is that of the moderator, and the spectral characteristics of the premoderator are essentially invisible.

Another interesting aspect of composite moderators is the fact that the thin liquid hydrogen layer might be easily removable, leaving one with a thick, conventional water moderator. So, an experiment could be repeated at the same instrument with a pure water spectrum, then a composite moderator spectrum. One could even envisage having the hydrogen layer divided into two or more sub-layers e.g., by having a number of thin canisters, and fill these canisters progressively with liquid hydrogen to produce more and more colder neutrons and therefore change the spectral characteristics of the neutron beam.

Energy deposition in moderators

The work described here gives quantitative estimates of the impact of proton beam shape and location on energy deposition in the existing liquid hydrogen moderator at LANSCE. More precisely, we describe below the results of two sets of studies:

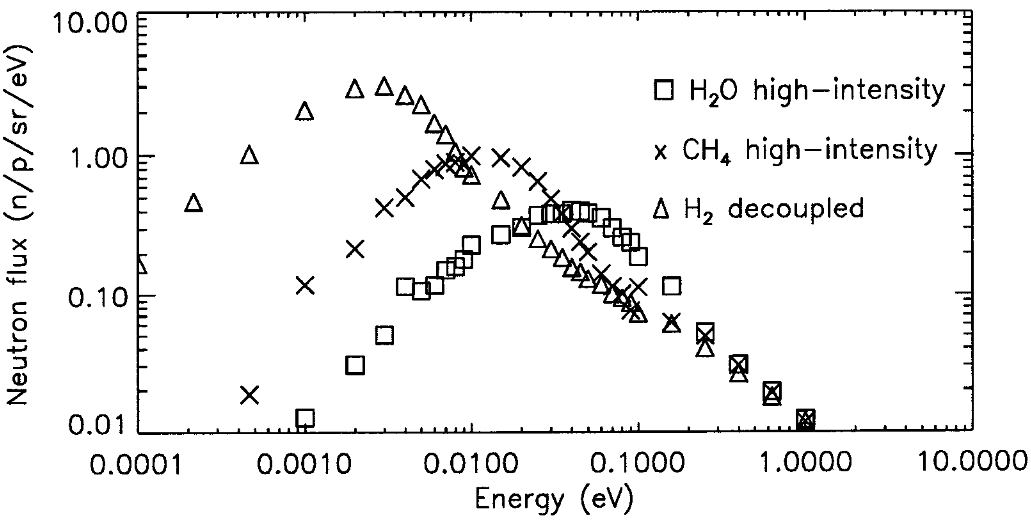
- Influence of the proton beam shape on moderator and target heating.
- Energy deposition in the cryogenic (liquid hydrogen) moderator and in the targets for various beam configurations.

In each case, energy deposition in the moderators was calculated for the moderating medium as well as for the aluminum canisters containing the moderator itself.

The results were obtained with the LAHET Code System (LCS) [6]. We used a detailed computer model of the as-built LANSCE target station created by X-6, and further developed at LANSCE. Fig.4 shows the exact geometry used in our calculations; more details can be found in Ref.[7].

First set of studies : Proton beam shape

Previous studies seem to indicate that at the 5% (or less) level, the exact beam shape does not matter much as far as neutron production is concerned (at least not as long as most of the beam reaches the target) [8]. Energy deposition in the moderators and targets, however, is rather sensitive to the exact location and shape of the proton beam.



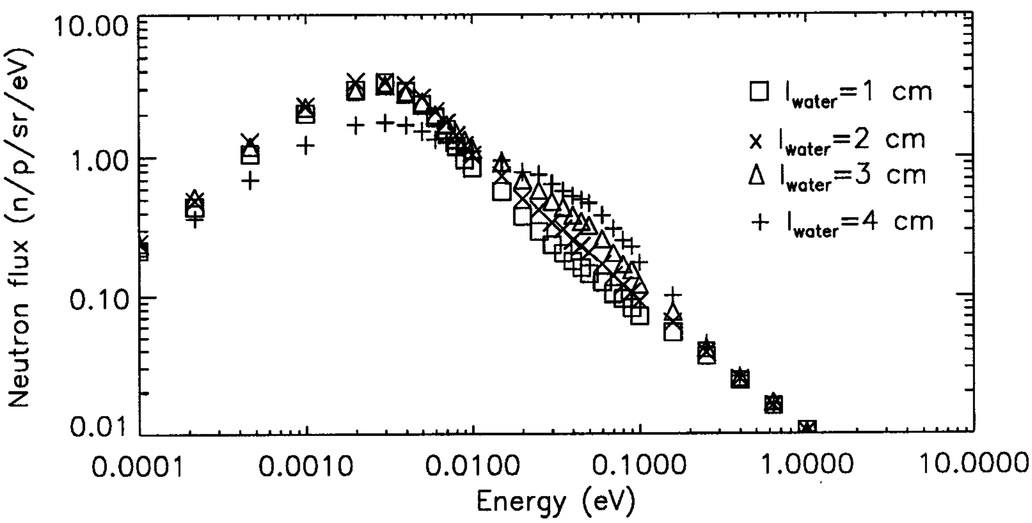
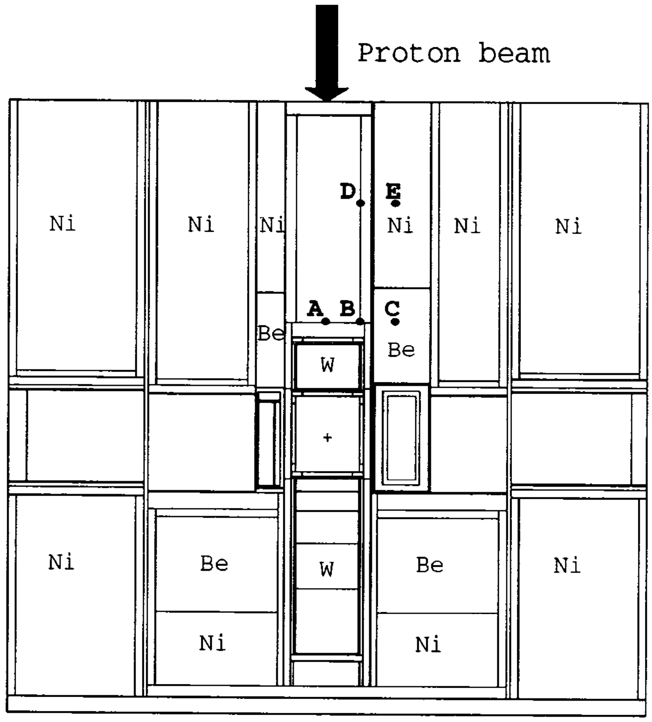


Figure 3: The top figure shows typical moderator spectra for liquid hydrogen, liquid methane, and light water moderators. The spectra were obtained for the moderators in flux trap geometry as described in the preceding section. The bottom figure shows composite moderator spectra for the light water/liquid hydrogen composite moderator described in the text. The total thickness of the moderator (water + liquid hydrogen) is fixed at 5 cm. Notice how the water spectrum emerges as the thickness of the liquid hydrogen layer is reduced. Compare the spectrum corresponding to $l_{water} = 4$ cm to the liquid methane spectrum in the top figure.



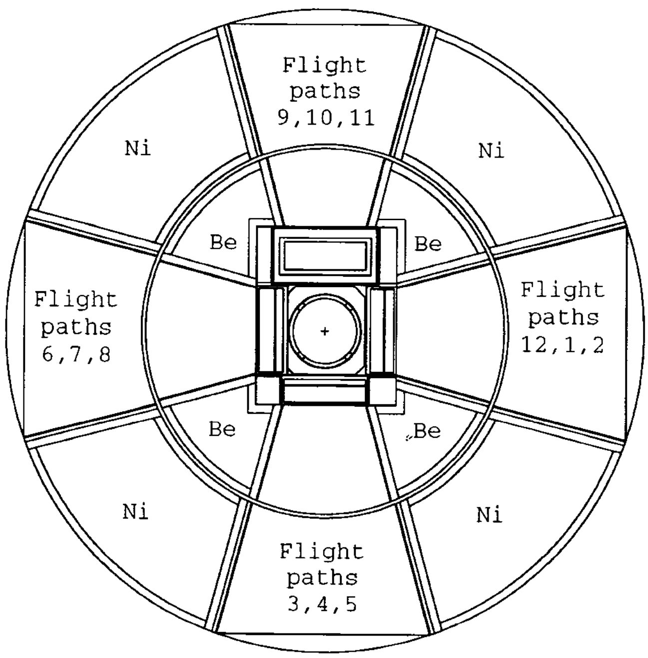


Figure 4: Computer model of the as-built LANSCE target station.

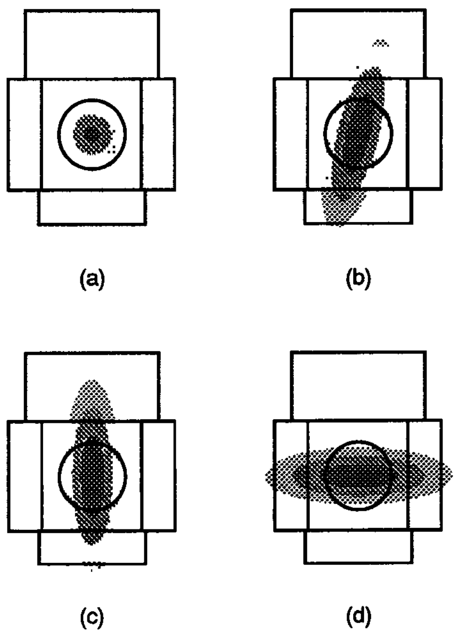


Figure 5: Beam spot shapes

In what follows, we assume that the beam is centered on target, and we vary its shape. Ideally, a circular beam spot on target would probably be the best situation one could imagine, Fig.5(a). Except for beam profile effects, target heating would be uniform azimuthally with no temperature gradients other than radial and axial gradients. Past experience at LANSCE has shown that if the proton beam is focussed to create a circular beam spot on target, the centerline thermocouples in the upper target register rather large temperatures, but energy deposition in the cryogenic moderator decreases. The beam was therefore defocussed to reduce centerline temperatures to acceptable levels. So far, we have not been able to reconcile in a fully satisfactory manner theoretical calculations of target temperatures with the measured temperatures. An effort is underway to explore systematically beam spot shapes effects. The results described below originate from studies performed in support of this effort.

The current production beam spot at LANSCE is assumed to be elliptical [9]. The beam profile is approximately Gaussian. The standard deviation along the semi-major axis and semi-minor axis of the ellipse are $\sigma_x = 3.8$ cm and $\sigma_y = 1$ cm, respectively, as measured by the thermocouples array above the target window. The semi-major axis is rotated (clockwise) 15^o with respect to the normal to the viewed surface of the cryogenic moderator, Fig.5(b).

In our computer studies, we simulated these two situations, as well as the situation shown in Fig.5(c). In all cases, the beam was centered on target. The beam profile was cut off at three standard deviations, i.e., the beam spot is an ellipse with semi-major axis and semi-minor axis equal to 11.4 cm and 3 cm, respectively. The beam was started at the top of the LANSCE reflector/shield. Notice that the beam is somewhat too wide to fit inside the beam hole, and is therefore truncated by the reflector/shield. Most protons reach the target nonetheless because 86.47 % of the protons are contained within 2 standard deviations (and this fits easily in the beam hole). Some high-energy protons hit the reflector as may be the

(a) Cell	Energy deposition High-energy particles (MeV/p)	Energy deposition Low-energy n (MeV/p)	Energy deposition γ rays (MeV/p)	Total (MeV/p)	Power Density (W/l/μA)
Moderators					
(12,1,2)	0.573	0.665	0.217	1.454	2.177
(3,4,5)	0.562	0.632	0.187	1.381	2.202
(6,7,8)	0.721	0.717	0.222	1.659	2.397
(9,10,11)	0.0597	0.368	0.0201	0.448	0.596
Al canisters					
(12,1,2)	0.567	0.0502	0.248	0.865	2.688
(3,4,5)	0.570	0.0467	0.199	0.816	2.587
(6,7,8)	0.710	0.0519	0.218	0.980	3.017
Inner (9,10,11)	0.553	0.0561	0.293	0.902	1.801
Outer (9,10,11)	0.411	0.0394	0.239	0.690	2.048
Targets					
Upper	246.203	0.484	14.839	261.5	475.6
Lower	204.263	0.375	15.667	219.3	103.4

Table 2: Energy deposition for the beam profile shown in Fig.5(a)

case in practice.

Tables 2-4 summarize the results of our computer study. In particular, the study confirms that the heat load in the cryogenic moderator decreases when going from the production beam to a circular beam; energy deposition in the target increases. The energy deposited in each cell is the sum of three contributions: The high-energy contribution includes heating from inelastic scattering of high-energy ($>$ 20 MeV) primary and secondary particles; The low-energy ($<$ 20 MeV) contributions include inelastic scattering of low-energy neutrons, and gamma-ray heating.

The variations in energy deposition either in the targets or in the moderators are rather modest, of the order of 10 to 20 %. Although not dramatic, these changes could affect a cooling system that is running close to its capacity. Finally, it is probably useful to emphasize that the energy deposition from high- or low-energy particles is virtually instantaneous compared to the time scale involved for a refrigeration or cooling system to react to a rapidly changing heat load.

Second set of studies : Beam location

The purpose of this study was to investigate the impact of beam location on target on the heat load in targets and moderators. More specifically, we considered extreme conditions where, for instance, the proton beam is directed directly to the cryogenic moderator, or hits the walls of the proton beam hole halfway down the hole, above the cryogenic moderator. These proton beam steering scenarios are somewhat extreme, but they set an upper bound on the heating conditions that may exist in the targets and moderators at LANSCE.

In order to simulate a worst case situation for the hydrogen moderator when the proton beam is directed above it, we used the beam spot shown in Fig.5(d) rather than the production beam spot. The preceding set of studies has shown that there is little difference between the beam spots shown in Figs.5(b), (c), or (d) anyway. Furthermore, in order to make the situation

(b) Cell	Energy deposition High-energy particles (MeV/p)	Energy deposition Low-energy n (MeV/p)	Energy deposition γ rays (MeV/p)	Total (MeV/p)	Power Density (W/l/μA)
Moderators					
(12,1,2)	0.536	0.630	0.208	1.374	2.058
(3,4,5)	0.640	0.617	0.204	1.440	2.296
(6,7,8)	0.679	0.674	0.218	1.571	2.270
(9,10,11)	0.0915	0.369	0.0756	0.481	0.640
Al canisters					
(12,1,2)	0.525	0.0467	0.238	0.810	2.517
(3,4,5)	0.762	0.0490	0.198	1.009	3.199
(6,7,8)	0.641	0.0495	0.206	0.897	2.761
Inner (9,10,11)	0.765	0.0550	0.294	1.114	2.224
Outer (9,10,11)	0.557	0.0405	0.236	0.834	2.476
Targets					
Upper	237.882	0.442	13.589	251.9	458.2
Lower	189.622	0.345	14.646	211.3	99.6

Table 3: Energy deposition for the beam profile shown in Fig.5(b)

(c) Cell	Energy deposition High-energy particles (MeV/p)	Energy deposition Low-energy n (MeV/p)	Energy deposition γ rays (MeV/p)	Total (MeV/p)	Power Density (W/l/μA)
Moderators					
(12,1,2)	0.566	0.622	0.208	1.396	2.091
(3,4,5)	0.668	0.613	0.189	1.471	2.345
(6,7,8)	0.673	0.664	0.215	1.553	2.244
(9,10,11)	0.0976	0.378	0.020	0.496	0.660
Al canisters					
(12,1,2)	0.546	0.0453	0.238	0.829	2.576
(3,4,5)	0.758	0.0471	0.204	1.009	3.199
(6,7,8)	0.687	0.0485	0.211	0.947	2.915
nner (9,10,11)	0.844	0.0568	0.285	1.186	2.368
Outer (9,10,11)	0.534	0.0405	0.236	0.811	2.407
Targets					
Upper	237.834	0.441	13.663	251.9	458.2
Lower	189.656	0.343	14.619	204.6	96.5

Table 4: Energy deposition for the beam profile shown in Fig.5(c)

A Cell	Energy deposition High-energy particles (MeV/p)	Energy deposition Low-energy n (MeV/p)	Energy deposition γ rays (MeV/p)	Total (MeV/p)	Power Density (W/l/μA)
Moderator (9,10,11)	0.0796	0.311	0.0168	0.407	0.541
Al canisters					
Inner (9,10,11)	0.500	0.0311	0.206	0.737	1.471
Outer (9,10,11)	0.586	0.0458	0.252	0.884	2.624
Targets					
Upper	192.783	0.349	11.075	204.2	371.4
Lower	160.927	0.301	13.137	174.4	82.2

Table 5: Energy deposition in the liquid H_2 moderator for proton beam at A, Fig.4

even worse, we started the beam right above the target, at different locations indicated by the letters A to E in Fig.4. So the beam is not truncated as it comes down the beam hole. Finally, we tried to spray as many high-energy protons as possible in the immediate vicinity of the targets and moderators by defocussing the beam further: The beam profile was cut off at 3.7 standard deviations (instead of 3 standard deviations).

The results are shown in Tables 5-9. Even when the beam is started right above the cryogenic moderator, although the energy deposited in the moderator is significantly larger, but not by several orders of magnitude – a factor of about 30 at most compared to a beam at location A. Notice that the situation corresponding to a beam at location C is not so far-fetched in practice. Indeed, the the cryogenic moderator is fed by a large pipe located directly above it, and running vertically parallel to the proton beam hole. This large pipe filled with liquid hydrogen provides a streaming path to the hydrogen moderator for any proton that hits the reflector in the vicinity of the pipe. We have made the requisite changes to our target computer model, and are in the process of testing this scenario. This situation is not limited to the hydrogen moderators: the other light-water moderators suffer from the same problem. The situation where the beam is started at location D is also a distinct possibility, should the beam drift towards the wall of the beam hole at some angle. Notice however that the effect is not particularly dramatic (if we ignore, for the sake of argument, the presence of the liquid hydrogen pipe just mentioned). The moderators are protected by the Ni and Be reflector/shield. The total length of Ni/Be above the moderators provides more than a stopping length for 800 MeV protons, thereby protecting the moderators against accidental excursions of the beam towards the moderators. The results for a beam started at location E confirm this.

Another interesting remark concerns the heat deposited in the moderating medium. From Tables 5-9, it is clear that the total energy deposited in the liquid hydrogen itself is a small fraction of the energy deposited in the entire moderator (Al canisters + liquid hydrogen). By far the largest amount of energy deposited in the moderator is deposited in the Al canisters. Of course, in practice, this energy is immediatly removed by the flow of liquid hydrogen in the inner canister, and it is the energy deposited in the liquid hydrogen plus the energy deposited in the inner canister that is considered in sizing the thermal capacity of the hydrogen circuit. The energy deposited in the outer canister is not so readily dissipated. It can only be dissipated by conduction through the sides of the canister that are directly in contact with the Be

B	Energy deposition	Energy deposition	Energy deposition	Total	Power
Cell	High-energy particles (MeV/p)	Low-energy n (MeV/p)	γ rays (MeV/p)	(MeV/p)	Density (W/l/μA)
Moderator (9,10,11)	0.240	0.241	0.0102	0.491	0.653
Al canisters					
Inner (9,10,11)	2.352	0.0400	0.151	2.543	5.077
Outer (9,10,11)	2.417	0.0293	0.128	2.574	7.641
Targets					
Upper	58.972	0.0944	5.150	64.216	116.8
Lower	63.605	0.114	8.074	71.793	33.9

Table 6: Energy deposition in the liquid H_2 moderator for proton beam at B, Fig.4

C	Energy deposition	Energy deposition	Energy deposition	Total	Power
Cell	High-energy particles (MeV/p)	Low-energy n (MeV/p)	γ rays (MeV/p)	(MeV/p)	Density (W/l/μA)
Moderator (9,10,11)	3.289	0.200	0.0066	3.496	4.650
Al canisters					
Inner (9,10,11)	31.839	0.0500	0.101	31.990	63.9
Outer (9,10,11)	7.507	0.0282	0.0830	7.618	22.6
Targets					
Upper	0.983	0.0530	2.945	3.933	7.154
Lower	11.678	0.0592	5.519	17.256	8.137

Table 7: Energy deposition in the liquid H_2 moderator for proton beam at C, Fig.4

D	Energy deposition	Energy deposition	Energy deposition	Total	Power
Cell	High-energy particles (MeV/p)	Low-energy n (MeV/p)	γ rays (MeV/p)	(MeV/p)	Density (W/l/μA)
Moderator (9,10,11)	0.289	0.208	0.0109	0.508	0.676
Al canisters					
Inner (9,10,11)	2.518	0.0366	0.163	2.718	5.426
Outer (9,10,11)	1.942	0.026	0.130	2.098	6.228
Targets					
Upper	65.818	0.106	3.844	69.8	127.0
Lower	55.967	0.101	5.760	61.8	29.1

Table 8: Energy deposition in the liquid H_2 moderator for proton beam at D, Fig.4

E	Energy deposition	Energy deposition	Energy deposition	Total	Power
Cell	High-energy particles (MeV/p)	Low-energy n (MeV/p)	γ rays (MeV/p)	(MeV/p)	Density (W/l/μA)
Moderator (9,10,11)	0.0362	0.0616	0.0062	0.104	0.138
Al canisters					
Inner (9,10,11)	0.337	0.0105	0.0904	0.438	0.874
Outer (9,10,11)	0.243	0.0075	0.0649	0.315	0.935
Targets					
Upper	0.0929	0.0017	1.183	1.278	2.235
Lower	0.396	0.0051	1.195	1.596	0.753

Table 9: Energy deposition in the liquid H_2 moderator for proton beam at E, Fig.4

reflector. If anything, this outer canister is the likely candidate for damage following a proton beam excursion. However, even in the worst case described above (location C), there seems to be enough heat conduction to keep the outer Al canister at a temperature well below the temperature range where structural damage to the material would compromise its mechanical integrity.

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