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THE BACKSCATTERING SPECTROMETER HERMES: DESIGN ISSUES

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1. Introduction

A computer model of the backscattering spectrometer HERMES was used to help answer a number of issues that arose during the conceptual design of the spectrometer. In particular, the performance of the spectrometer was evaluated on several types of moderators:

- A decoupled liquid hydrogen moderator;
- A partially coupled liquid hydrogen moderator;
- A decoupled, poisoned liquid hydrogen moderator.

Variying the degree of coupling of the moderator to the reflector , as well as poisoning the moderator can affect greatly the time and energy distribution of the neutron pulse emitted by the moderator. The proposed reflector for the LANSCE upgrade is a composite reflector made of beryllium in the immediate vicinity of the moderators. A second layer of lead completes the reflector and surrounds the inner reflector/moderators assembly.

The main purpose of the reflector is to reflect toward the moderators neutrons that would otherwise have missed the moderators and give these neutrons a second chance at moderation. While beryllium is a good reflecting material, it is also a good moderator. Therefore, in addition to returning fast (epithermal and faster) neutrons to the moderator, it also returns a large moderated neutron flux long after the target was pulsed. This increases the (time-integrated) intensity of the emitted neutron pulse, but it does so at the expense of adding a long tail to the pulse.

One can mitigate this effect by establishing a barrier between the moderator and the reflector. This barrier, a decoupler, is a material that strongly absorbs neutrons in the thermal range but is more or less transparent to faster neutrons. In this way, the reflector can only return fast neutrons to the moderator. The moderated (thermal) component of the flux returned at later times by the reflector to the moderator is eliminated. Typical decoupling materials are cadmium, gadolinium, and boral -an alloy of aluminum and boron-10. Notice that it is possible to vary the degree of coupling (or decoupling) by adjusting the thickness of the decoupler, as well as by completely or partially isolating the moderator and the reflector. The proposed partially coupled liquid hydrogen moderator for the LANSCE upgrade is not directly decoupled with any material. Its back is surrounded by the other three moderators which are decoupled. This arrangement prevents the three water moderators from returning thermal neutrons to the liquid hydrogen moderator. The flight path penetration facing the moderator does not have its walls covered with decoupling materials so that the moderator face "views" the reflector directly.

It is possible to further sharpen the pulse by poisoning the moderator. This operation consists in introducing a sheet of material such as gadolinium inside the moderator to absorb neutrons that spend too much time thermalizing in the moderator. This, effectively, produces a significantly sharper pulse at the expense of some loss of intensity.

2. Moderator Characteristics

Figure 1 shows the wavelength-emission time distribution for the three moderators mentioned above. It is clear from Figure 1 that coupling the moderator to the reflector, even partially, has a dramatic effect on the neutron pulse. Notice that in Figure 1 intensity is given in absolute units and the scale is the same for all three figures.

The pulses shown in Figure 1 were used as source terms in the Monte Carlo simulations. They are a fit to an analytical form of data obtained from a radiation transport code, MCNP, for which a detailed model of the LANSCE neutron production target station is available. The general analytical form, proposed by Ikeda and Carpenter, to represent the neutron emission time-velocity distribution of the neutron pulse is [1]:

$$\psi(\lambda,t)=\int dt'\phi(\lambda,t')\left[(1-R)\left[(1-q)\delta(t-t')+q\exp\left(-\frac{(t/\lambda)}{(t/\lambda)_0}\right)\right]+\frac{R}{\tau}\theta(t-t')\exp\left(-\frac{t-t'}{\tau}\right)\right], \tag{1}$$

where δ is the Dirac delta function, θ is the step function, $(t/\lambda)_0$ and $0<q<1$ are fitting parameter, τ is the pulse decay time constant, $R=\exp(-\lambda_0^P/\lambda^P)$ is a joining function (P and λ_0 are fitting parameters). The function ϕ is given by:

$$\phi(\lambda,t)=\frac{1}{2\alpha\lambda}\left(\frac{t}{\alpha\lambda}\right)^2\exp\left(-\frac{t}{\alpha\lambda}\right), \tag{2}$$

where α is yet another fitting parameter. In the above equation, $t>0$. Strictly speaking, the Ikeda-Carpenter equation corresponds to $q=0$. The additional parameter, q, allows a better fit to the data in certain regions of the (λ,t)-space. The convolution integral is easily calculated numerically or analytically. The first term in the equation for ψ represents basically the early part of the neutron pulse while the second term represents the exponential decay of the pulse at longer times. The quantity ψ is normalized so that integration over all λ and all $t>0$ yields unity.

The (time-averaged) spectrum was taken directly from the MCNP simulation and added to the source file as a table. No attempt was made to fit the spectrum to an analytical expression such as that used in Ref.[1]. Figure 2 shows the neutron energy spectrum between 0.1 meV and 10 meV for the three moderator considered in the present study. Table 1 below summarizes the main characteristics of the moderators used in the Monte Carlo studies.

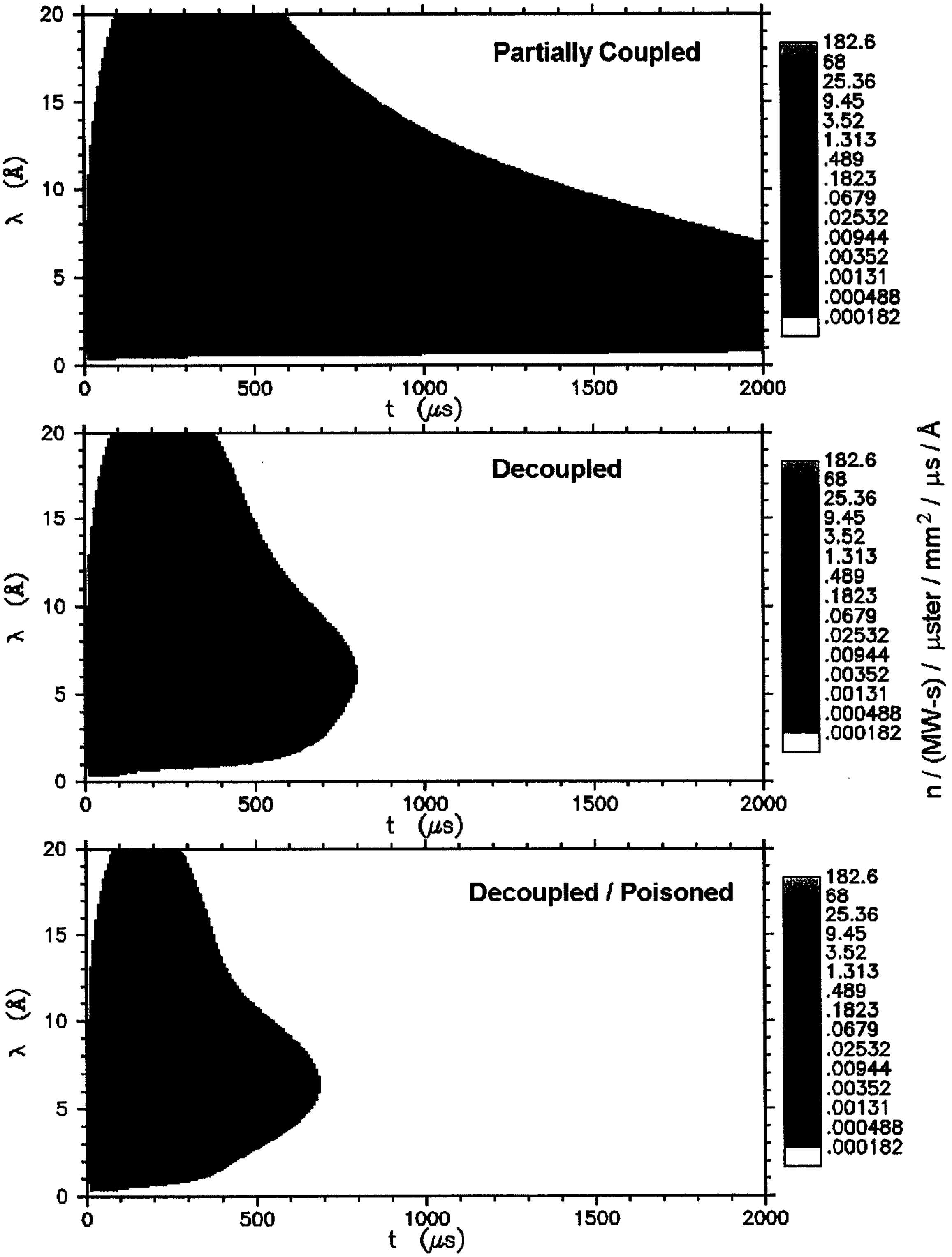

Figure 1. Emission time-Wavelength distribution function corresponding to the three liquid hydrogen moderators considered in this study. (A note on units: the flux is normalized per mm^2 of moderator surface area, per μs of emission time, per Angstrom, per μster, and per MW.s. The latter refers to the (time-averaged) energy deposited by 800 MeV protons in the neutron production target in 1 second. In order to obtain a flux per pulse, divide by the source frequency. To normalize to a 200 μA, 800 MeV proton beam, multiply by the beam power, 0.160 MW.)

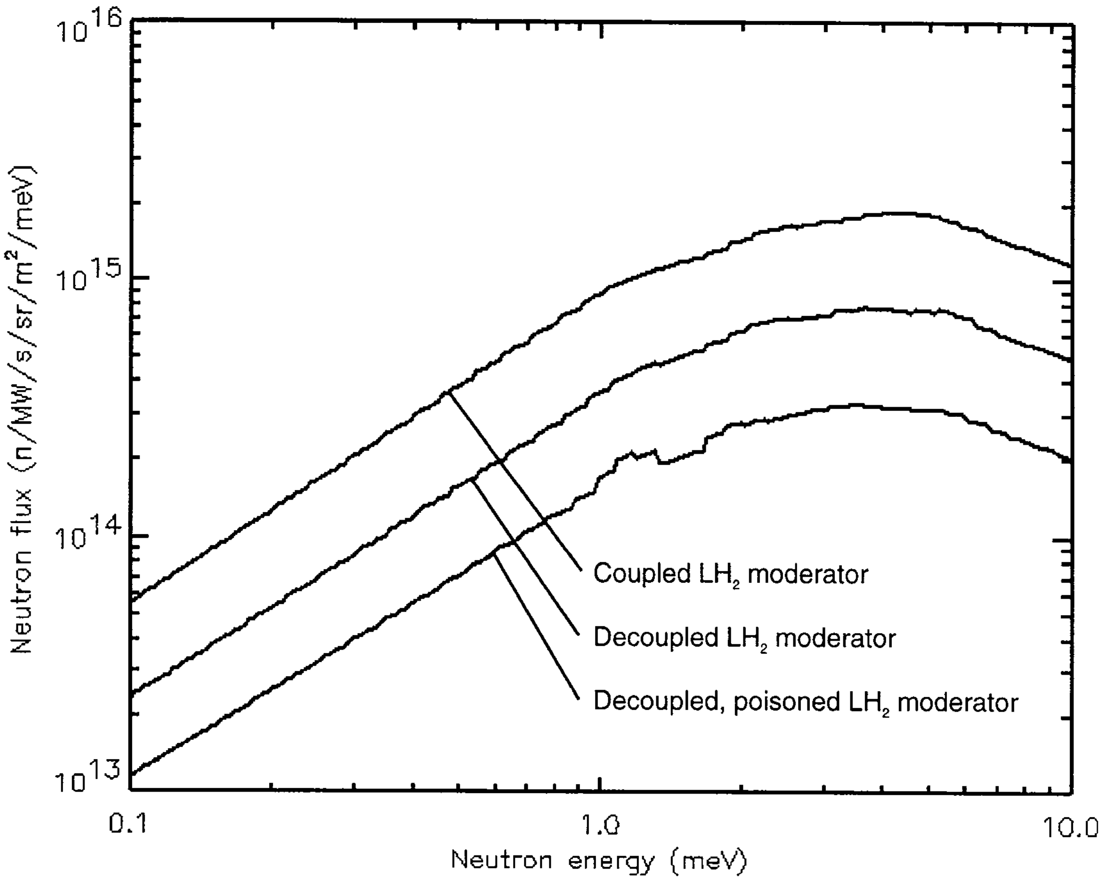

Figure 2. The (time-averaged) neutron energy spectrum for the three moderators considered in our study.

Table 1. Essential characteristics of the moderators used in our study.

MODERATING MEDIUM	**LIQUID H_2 @ 20K**	**LIQUID H_2 @ 20K**	**LIQUID H_2 @ 20K**
Thickness	5 cm	5 cm	5 cm
Size	12 x 12 cm^2	12 x 12 cm^2	12 x 12 cm^2
Decoupler, liner	Cd	Cd	None
Poison	Gd (17 mils), 2.5 cm depth	None	None
Surface current (0.1-5 meV range)	1.24x10^{15} n/sr/m^2/MW/s	2.89x10^{15} n/sr/m^2/MW/s	6.87x10^{15} n/sr/m^2/MW/s
Peak intensity @1.8 meV	3.30x10^{18} n/sr/m^2/μs/meV/MW/s	4.34x10^{18} n/sr/m^2/μs/meV/MW/s	5.47x10^{18} n/sr/m^2/μs/meV/MW/s
FWHM of pulse shape	80.0 μs	100.5 μs	152.0 μs
Exponential decay time constant(s)	54.5 μs	84.5 μs	100.0 μs, 400.0 μs
Rise time (10-90 %) @ 1.8 meV	24 μs	30 μs	35 μs

Table 2. Moderator parameters at 1.8 meV. The coupled moderator has one more parameter, q'=60%.

Moderator	α (μs/A)	$(t/\lambda)_0$ (μs/A)	λ_0(A)	P	Q(%)	τ_1 (τ_2) (μs)
Decoupled, poisoned	2.83	20.5	6	0.9	31.9	54.2
Decoupled	3.11	20.6	4.6	1.1	30.9	84.0
Coupled	2.0	15.0	1.5	1.79	25.0	100.0 (400.0)

From Figure 2, we see that the neutron flux for the partially coupled moderator is a factor of 5.5 larger than that that for the decoupled poisoned moderator, and a factor of 2.4 larger than the flux from the decoupled moderator. There is a factor of 2.3 in intensity between the decoupled moderator and the decoupled, poisoned moderator. The moderator pulse shape parameters at 1.8 meV are given in Table 2.

3. Monte Carlo Simulations

The Monte Carlo simulations were performed with the LANSCE Neutron Instrument Simulation Package (NISP). Most of the parameters for the simulation are easily set with the exception of parameters for the crystal analyzers. The NISP model for monochromating crystals requires one to give the lattice spacing, d, for the crystal, as well as the statistical distribution of d. While the former is well-known for pyrolytic graphite, the latter is more problematic. NISP allows the user to use a Gaussian or a Lorentzian for the statistical distribution of d, and there remains to choose a value of the standard deviation or the full width at half-maximum for the Gaussian or Lorentzian, respectively. We chose a Lorentzian distribution and set the value of the full width at half-maximum of the distribution by attempting to reproduce the elastic line shape produced by a vanadium sample (incoherent, elastic, isotropic scatterer) at the IRIS backscattering spectrometer. The reason behind this somewhat complicated way of determining the full width at half-maximum, Δd, is that its value is not known with great accuracy for graphite. A typical value, quoted by manufacturers, of $\Delta d/d$ is anywhere from $1.5\text{x}10^{-3}$ to $2\text{x}10^{-3}$ [2]. Similarly, the mosaic spread of graphite crystals is not known very well. The instrument resolution, however, is much less sensitive to this parameter which was fixed to the nominal value specified by the manufacturer. All other parameters were fixed to the appropriate values for IRIS. The primary flight path length is 36.41 m; the analyzer radius is 0.85 m; the height of the analyzer is 0.06 m; the angle of incidence on the analyzer crystals is 88.5^{o}; and we used the decoupled moderator described above as our source term. This moderator, while calculated with the LANSCE target station model, has essentially the same characteristics as the ISIS liquid hydrogen moderator: a full width at half-maximum of the neutron pulse at λ=6.70 Angstrom of 120 μs and a decay time constant of about 84 μs.

The result is shown in Figure 3. The Monte Carlo simulation reproduces the IRIS vanadium data very well. It should be noted however that we had to use a value of $\Delta d/d$ of about $1\text{x}10^{-3}$ to obtain good agreement. This value is smaller than that quoted by the manufacturer. This may not be all that surprising since the graphite crystals used for the IRIS analyzer were tested individually and the better quality crystals (lower value of ?d/d) were selected systematically. The entire set of crystals should thus have an average value of $\Delta d/d$ that is smaller than the value of $2\text{x}10^{-3}$ quoted by the manufacturer [2].

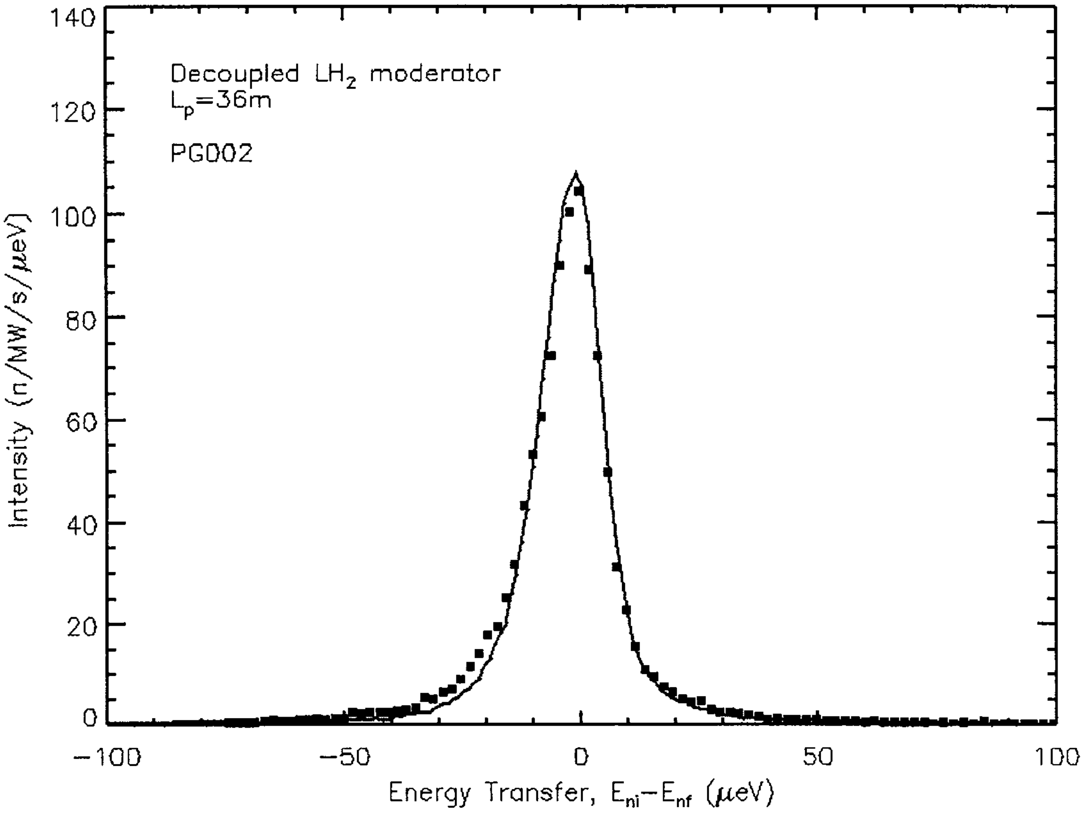

Figure 3. A comparison between the elastic line shape measured at IRIS with a vanadium sample and the results of a corresponding Monte Carlo simulation with NISP. The full width at half-maximum of the elastic line is about 14 μeV. The moderator used in this study is the decoupled moderator. This moderator has characteristics very similar to those of the ISIS liquid hydrogen moderator. These characteristics are summarized in Table 1.

In Figure 3, the calculated line shape agrees quite well with the experimental measurement, particularly for positive (neutron) energy transfers. The agreement is not quite as good for negative (neutron) energy transfers. This may be due to the fact that the neutron pulse used in the simulation corresponds to a decoupled liquid hydrogen moderator at the LANSCE target station. (A source file for the ISIS liquid hydrogen moderator is not available.) Nonetheless, the moderator used has the same full width at half-maximum (120 μs at 1.82 meV) as the IRIS liquid hydrogen moderator. The decay time constant is not known very accurately, but it would appear that the value of 84 μs corresponding to the LANSCE moderator used is fairly close to the actual value. A somewhat better agreement could be obtained by adjusting this value to a slightly smaller number, but we did not pursue this. The (energy-integrated) count rate at IRIS is approximately 335 n/s in the detector bank facing the graphite analyzer.

4. Decoupled Liquid Hydrogen Moderator

The moderating medium is liquid hydrogen at 20 K. The moderator is decoupled with cadmium on all sides except the moderator face and the corresponding flight path is also lined with cadmium. In our simulations, we focussed mainly on the use of the graphite 002 line at the analyzer, i.e., we are interested in neutron wavelengths around 6.7 Angstrom (1.82 meV). Table 1 above summarizes the main features of the liquid hydrogen moderator. This moderator was used as a source in a Monte Carlo simulation of HERMES. The basic characteristics of the simulated instrument are:

- Primary flight path: 36 m
- Analyzer: Pyrolytic graphite mounted on equatorial strip of spherical surface
- Analyzer radius: 0.85 m
- Analyzer height: 0.3 m
  - Sample: isotropic, elastic delta scatterer
  - Analyzer: mica and graphite

The use of an idealized isotropic, elastic delta scatterer allowed us to determine the elastic resolution of the instrument. This is shown in Figure 4 where the elastic line shape calculated with the Monte Carlo package NISP appears together with the experimentally measured IRIS line shape (scaled to match the peak value of the Monte Carlo calculations). The agreement between the calculated elastic peak and the measured one is very good. Both have a full width at half-maximum of about 14 μeV.

Notice that in Figure 4, intensity is given in absolute units (n/MW/s/μeV). At a proton beam power of 160 kW, the (energy-integrated) count rate in the detector on the graphite side of the analyzer is approximately 1376 n/s. This count rate is 4.1 times that of IRIS. This is consistent with the fact that the analyzer height is five times larger (30 cm) in the present HERMES design than it is in the IRIS instrument (6 cm).

5. Partially Coupled Liquid Hydrogen Moderator

As described above, the proposed partially coupled liquid hydrogen moderator for the LANSCE upgrade has a piece of decoupler on its back, the sides have no decoupler, and the flight path is not line with decoupling material. This moderator is thus quite strongly coupled to the reflector. In order to obtain a reasonable fit to an Ikeda-Carpenter-like formula, one has to split the exponential decay term at longer times into a linear combination of two exponential terms with decay constant τ_1 and τ_2:

$$\exp\left(-\frac{t-t'}{\tau}\right) \rightarrow q'\exp\left(-\frac{t-t'}{\tau_1}\right) + (1-q')\exp\left(-\frac{t-t'}{\tau_2}\right) \qquad (3)$$

where $0<q'<1$.

At 160 kW proton beam power, the estimated (energy-integrated) count rate at the detector bank facing the graphite analyzer is approximately 3109 n/s. It is larger (by a factor of 2.25) than the 1376 n/s count rate calculated for the decoupled moderator. If we compare the peak count rates (70.4 n/s/μeV for the decoupled moderator; 118.8 n/s/μeV for the coupled moderator -a factor of 1.65 difference), however, it is evident that the increased count rate (integrated over energy) is due largely to the broadening of the elastic line and the addition of a tail at negative neutron energy transfers.

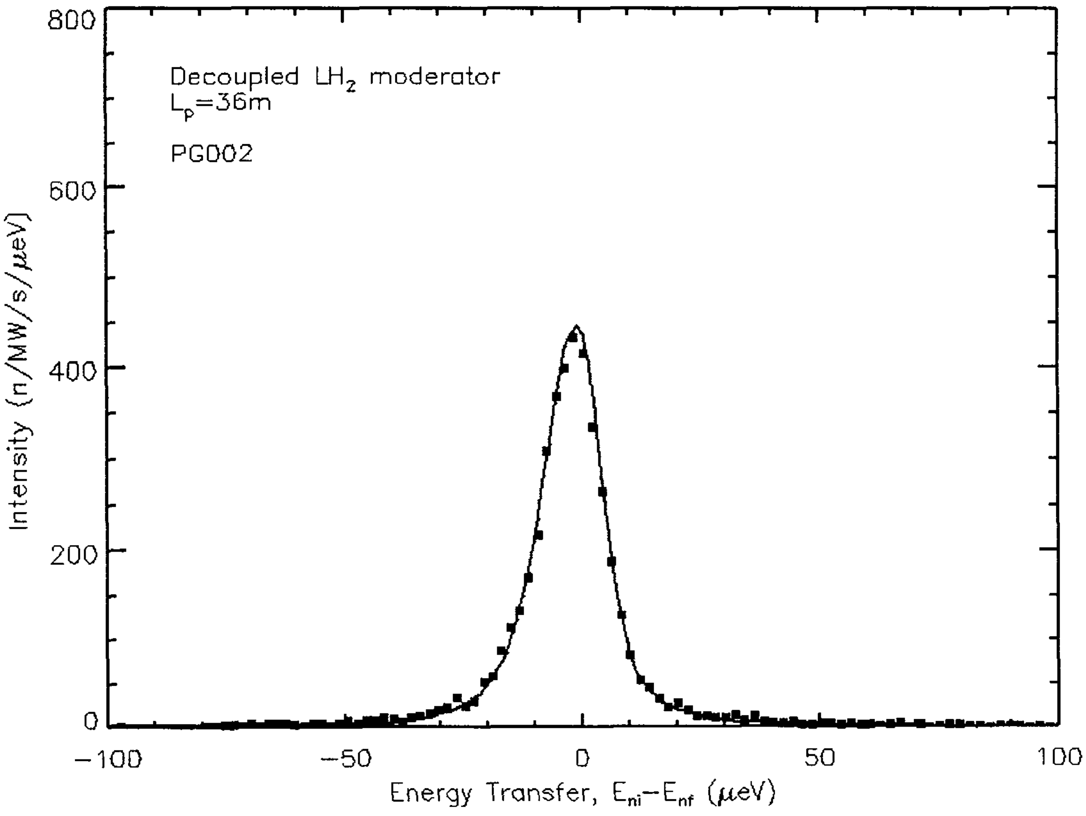

Figure 4. The elastic line shape calculated for a 36 m long instrument with a 0.3 m high analyzer (squares). The solid line is the experimentally-measured IRIS line shape scaled in magnitude to match the peak value of the Monte Carlo result. The full width at half-maximum of the elastic line is 14 μeV. The higher intensity (compared to Figure 3) is due to the larger analyzer height (0.3 m v. 0.06 m at IRIS).

It would appear at first sight that the long tail is the one feature of the neutron pulse that most affects the elastic line and that the decoupled moderator with a shorter decay time constant would be more desirable. Indeed, one may ask whether the presence of the long tail in the elastic resolution function is detrimental to the determination of small inelastic peak near the elastic line, or even to the analysis of a quasielastic spectrum. To resolve this issue, it will be necessary to perform a complete data analysis on the output of the Monte Carlo simulations.

6. Decoupled, Poisoned Liquid Hydrogen Moderator

One can further reduce the neutron pulse width by poisoning the moderator. In this calculation, we placed a 0.508 mm (17 mils) thick foil of gadolinium in the middle of the decoupled moderator. The main characteristics of the pulse are listed in Table 1. As mentioned previously, the effect of the poison is to reduce the FWHM of the neutron pulse at thermal and sub-thermal energies. This happens at the cost of sacrificing peak and integrated intensity.

Figure 6 shows the Monte Carlo-calculated elastic line shape for the decoupled poisoned moderator. Despite the relatively narrow neutron pulse (FWHM = 80 μs -compare with the decoupled, non-poisoned moderator for which FWHM = 100 μs), the FWHM of the elastic line is virtually the same, namely 12 μeV (14 μeV for the decoupled, non-poisoned moderator). This seems to indicate that at a length of 36 m, the resolution gain to be made by using a narrower neutron pulse is quite modest indeed. The resolution is dominated by the non-zero backscattering angle and/or by the distribution of lattice spacings in the analyzer graphite crystals.

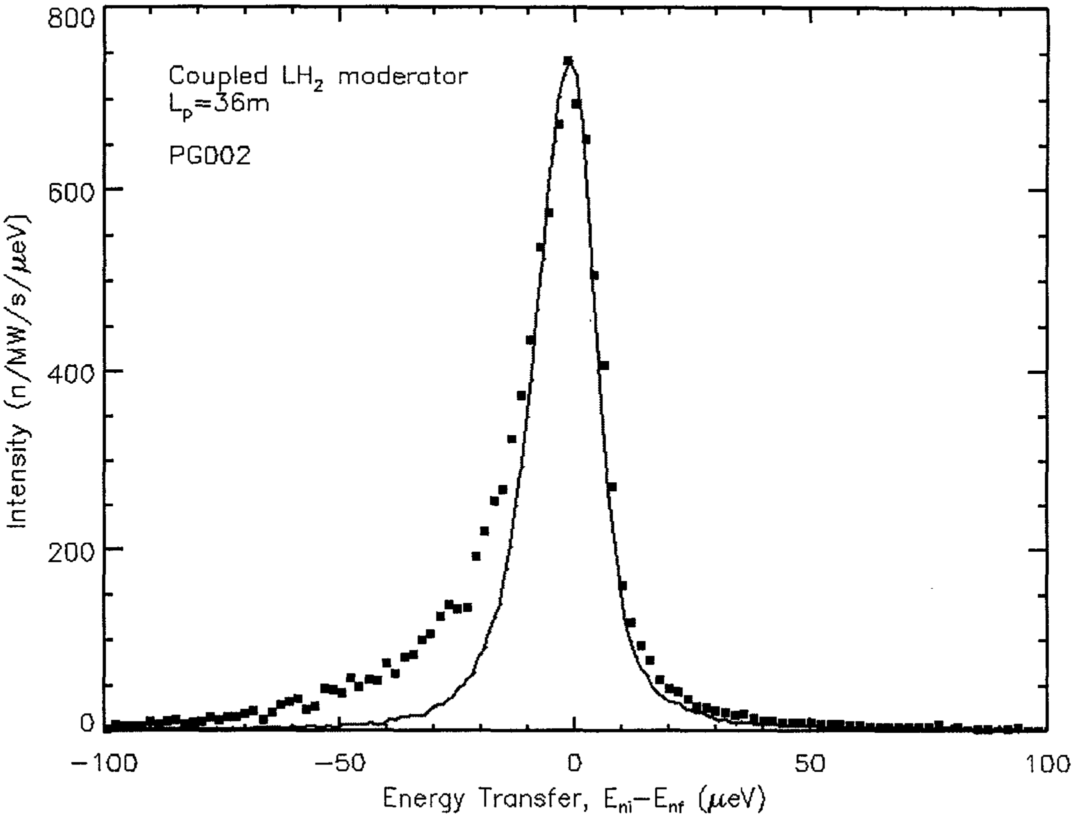

Figure 5. The calculated elastic line shape (squares) for the partially coupled liquid hydrogen moderator. The full width at half-maximum of the calculated elastic line shape is17.5 μeV. Also shown for comparison is the elastic line shape at IRIS (solid line, FWHM = 14 μeV). The large asymmetry introduced by the presence of a long tail in the neutron pulse is clearly visible.

The elastic line shape, however, is nicely symmetric with a FWHM comparable (slightly smaller) to that measured on the IRIS instrument at the Rutherford-Appleton Laboratory (U.K.).

The (energy-integrated) count rate at the detector (on the graphite side of the analyzer) is now about 587 n/s, significantly lower than the count rate of 1376 n/s calculated for the decoupled (non-poisoned) moderator, and somewhat larger than the IRIS count rate despite the analyzer surface area being 5 times that of IRIS.

7. Conclusion: Performance Comparison

Table 3 summarizes some of the results discussed above. Refer to it in the following discussion.

If we compare all three moderators, it would appear that the decoupled, non-poisoned moderator is ideal for HERMES.

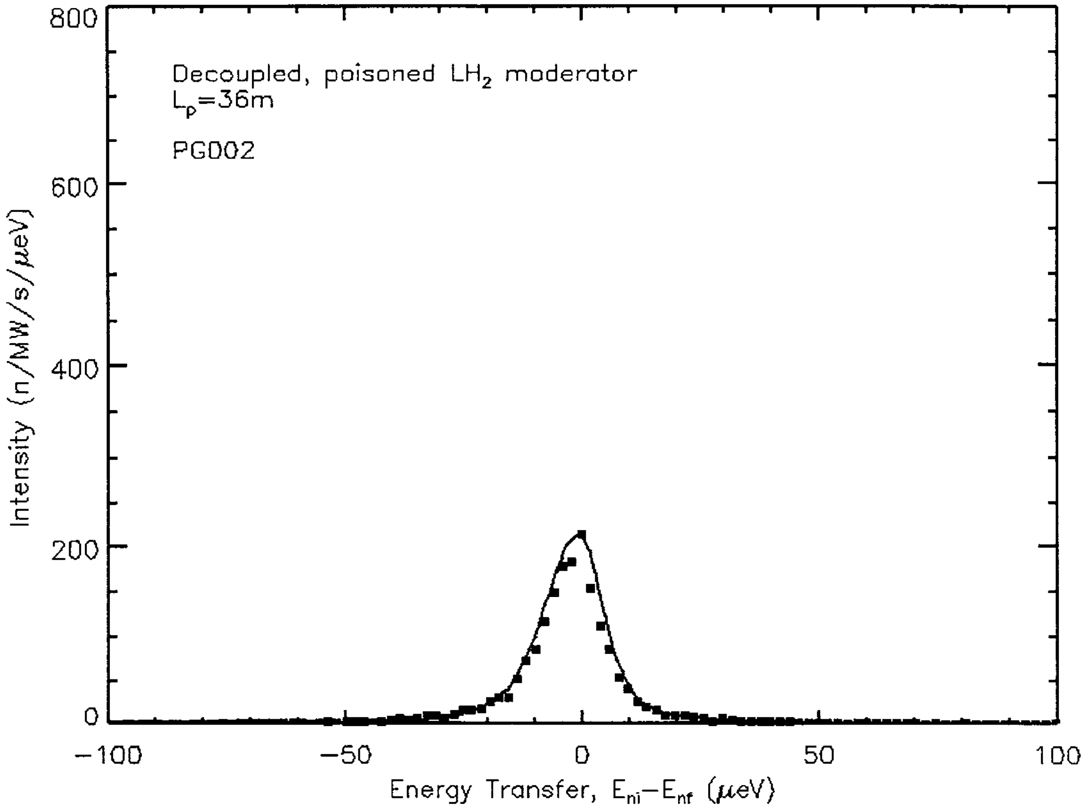

Figure 6. The elastic line shape for the decoupled, poisoned liquid hydrogen moderator. The FWHM of the peak from the Monte Carlo simulation (squares) is 12 μeV. The FWHM of the measured peak (solid line) is 14 μeV.

Indeed, the coupled moderator leads to a larger count rate (2.4 times the count rate for the decoupled moderator), but a significant fraction of the increase is due to an increase in line width and the addition of a tail to the elastic peak rather than an increase in peak intensity (which is a factor of 1.65 only).

The decoupled poisoned moderator leads to a very modest increase in line width at the cost of a decrease in count rate at the detector of a factor of about 2.3 compared to the decoupled, non-poisoned moderator case. This means that the pulse from the decoupled, non-poisoned moderator comes close to matching the backscattering angle and the Δd/d uncertainty for graphite on HERMES. No further gain in resolution can be achieved by means of using a narrower pulse. Instead, better resolution should be attained by using other crystals, e.g., mica, with a smaller value of Δd/d. For such crystals, it might be worth considering a decoupled poisoned moderator in order to further improve the elastic resolution of the instrument.

Comparison of Figure 3 and Figure 4 shows the intensity of the elastic line is about five times larger at the proposed HERMES instrument on a decoupled moderator than it is at IRIS. Yet, the FWHM of the peak is the same in both cases. The difference between the two simulations (besides a modest 41 cm difference in primary flight path) is the height of the analyzer: 30 cm on HERMES compared to 6 cm for IRIS. (The same moderator was used in both simulations.) Notice that the elastic line in Figure 4 remains highly symmetric.

Table 3. Performance comparison. Notice that the analyzer at HERMES has five times the height of the IRIS analyzer.

Instrument	**Moderator**	**FWHM (μs)**	**Count Rate (n/s)**	**Peak Count Rate (n/s/μeV)**
IRIS	Decoupled	14	335	16.7
HERMES	Decoupled, poisoned	12.5	587	34.2
HERMES	Decoupled	14	1376	70.4
HERMES	Coupled	17.5	3109	118.8

References

[1] S. Ikeda and J.M. Carpenter, *Nucl.Instr.Meth.*, **A239**, 536 (1985).
[2] C.J. Carlile and M.A. Adams, *Physica B*, **182**, 431 (1992).