ICANS-XIII
13th Meeting of the International Collaboration on
Advanced Neutron Sources
October 11-14, 1995
Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

# NEUTRONICS STUDIES FOR THE ESS SOURCE

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## ABSTRACT

This paper presents the results of calculations on two alternative target designs for the ESS pulsed spallation source. A conventional target based on the current ISIS design is compared with a split target incorporating both wing and flux trap moderators.

The results presented here focus on three issues, all of which are of general interest in the field of target-moderator systems. Firstly, the moderator performance is compared for the conventional and split target. For the purposes of the ESS study, the split target was found to offer no major advantage over a conventional target. Secondly, the variation of moderator performance with target diameter was examined. The results demonstrate that a flux trap moderator is significantly less sensitive to target diameter than wing moderators; thus a split target would be advantageous if a very large target diameter was found to be necessary. Thirdly, the performance of liquid para-hydrogen as a substitute for liquid methane (which would probably suffer unacceptable radiation damage on the ESS source) is evaluated. The results indicate that a suitably poisoned liquid $H_2$ moderator could be an acceptable substitute for a similar poisoned liquid $CH_4$ moderator.

## 1. Introduction.

This paper considers a fundamental issue in the design of a target for a pulsed neutron source. The calculations were performed primarily for the ESS study, but the results and conclusions are relevant to the design of any powerful spallation source.

A conventional spallation target consists of a single unit containing a high volume fraction of a heavy material, e.g. uranium or tantalum. For the purpose of maximizing neutron current, the best arrangement of moderators would be the 'slab' geometry (i.e. an arrangement similar to Fig. 2 without the target gap). However, this concept is normally rejected on the grounds that the beam lines view the target directly; it is widely believed that the resulting $\gamma$ and fast neutron backgrounds would be unacceptable. The geometry which is used in practice is the 'wing' geometry (see Fig. 3). This reduces the backgrounds by many orders of magnitude, at the cost of a reduction in moderator performance by about a factor of two.

Keywords: ESS, Spallation, Moderators, Target

An alternative design involves a split target divided into two or more sections. It is then possible to arrange moderators in a 'flux trap' geometry as in Fig. 2. Some of the advantages of slab geometry are then available, without the excessive backgrounds.

A second issue which this paper examines is the optimization of a cold moderator to be used in place of a poisoned liquid methane moderator as employed on ISIS and other current sources. Although the neutronic properties of liquid $CH_4$ are excellent, its susceptibility to radiation damage probably precludes its use on intense sources such as the ESS; liquid hydrogen, which is essentially immune to radiation damage, would be the best alternative.

## 2. Details of target and beam geometry

### *2.1 Conventional Target*

The model used for the conventional target is an approximate representation of the ESS tantalum target [1, 2]. For the purposes of our calculations the existing ISIS target-moderator-reflector geometry was used, with the proton energy increased to 1.334 GeV in accordance with the agreed value for the ESS study [3].

A horizontal section through the geometry is shown in Fig. 1. This shows the target, whose diameter is 10cm, and length 33.5cm, measured from the front of the first plate to the rear of the last. The target is flanked by 'cooling wings' represented by a homogenized mixture of stainless steel and heavy water, and a reflector represented by a homogenized mixture of beryllium and heavy water (80% Be, 20% $D_2O$ by volume).

Apart from the energy, the parameters of the proton beam were based on measured values for the ISIS target. A Gaussian profile was specified with $\sigma$=1.5cm and a cutoff radius of $3\sigma$, giving a beam diameter of 9cm.

### *2.2 Split Target*

For reasons of simplicity we proposed a two-component target incorporating both wing and flux trap moderators [4].

Figure 2 shows a horizontal section through the target-moderator-reflector configuration, the overall dimensions of which are an $80 \times 80 \times 80$ cm$^3$ cube. The lengths of the front and rear sections are 15cm and 20cm respectively, and the 'void' between the two target sections is 10cm. (Most of this space is a void; however, it contains two stainless steel windows, at the rear of the front target section and *vice versa*.) Details of the materials used in the calculation (as numbered in Fig. 2 is listed in Table 1.

Four calculations were performed with target diameters $D_T$ of 10cm, 12cm, 14cm and 16cm. In each case a parabolic beam profile was used with a beam diameter $D_B$ given by $D_B = D_T - 4$cm. A proton beam energy of 1.334 GeV was again specified.

For purposes of comparison the 10cm target was also run with the same beam profile as the conventional target: a 9cm diameter, a Gaussian profile and a $3\sigma$ cutoff.

## 3. Moderator design

### *3.1 Conventional Target*

A horizontal section through the upper moderators, all of which are in 'wing' geometry, is shown in Fig. 3. The lower moderators, which comprise an 'upstream' liquid methane moderator and a

Table 1: List of material numbers as used in the calculations for the split target geometry. Note: percentage compositions are by volume.

| Material No. | Description |
|---|---|
| 0 | Void |
| 3 | Light water |
| 5 | Be (70%) + $D_2O$ (30%) (homogenized reflector/coolant) |
| 6 | Gadolinium (moderator poison) |
| 7 | Cadmium (decoupler for $H_2$ flux trap moderator) |
| 11 | Liquid para-hydrogen |
| 14 | Boral (decouplers and liners) |
| 16 | Stainless steel (50%) + $D_2O$ (50%) (target pressure vessel and coolant, homogenized) |
| 18 | Tantalum (80%) + $D_2O$ (20%) (target material and coolant, homogenized) |

'downstream' liquid $H_2$ moderator, have a similar configuration below the target. Calculations were also performed for three alternative configurations in which the methane moderator was replaced by a liquid para-hydrogen moderator of thickness 6cm, 8cm or 10cm. Only the geometry of the moderator and its aluminium containers was varied; the boral and stainless steel decouplers and liners remained the same in all cases.

The parameters of the four moderators, and the three alternative liquid hydrogen moderators, are summarized in Table 2.

*3.2 Split Target*

The two pairs of moderators each consisted of a water moderator and a liquid hydrogen moderator (assumed to be pure para-hydrogen). The transverse dimensions of the moderators were $12 \times 12\text{cm}^2$ for the flux trap moderators, and $10 \times 10\text{cm}^2$ for the 'wing' moderators. Further information about the parameters of the moderators is given in table 3.

The arrangement of the flux trap moderators and their associated beam ports is shown in Fig. 2. There was one wing moderator of thickness 5cm with decoupler and poison above the front target module and below it there was a 10cm thick wing moderator with no decoupler or poison.

In all cases the upper and lower boundaries of the beam ports were specified as parallel, horizontal surfaces. However, the vertical surfaces were made to diverge at an angle of 15° relative to a direction normal to the target axis.

## 4. Computational details

The calculations were performed using the LCS suite of codes [5]. The code LAHET was used for the high energy calculation ($>$ 20MeV), and the neutron transport calculation was continued down to thermal energies using the code HMCNP4A, a version of MCNP modified to interface

Table 2: Moderator parameters for the conventional target. (Dimensions in cm. except where stated. Decouplers are equidistant from the two moderator faces unless otherwise stated.)

| **Moderator** | **Dimensions ($cm^3$)** | **Decoupler** | **Poison** |
|---|---|---|---|
| $H_2O$ (upstream) (300K) | 12.5 × 12.0 × 4.5 | 6.5mm Boral | 2 × .025mm Gd (each 1.05cm from nearest face.) |
| $H_2O$ (downstream) (300K) | 12.5 × 12.0 × 4.5 | 6.5mm Boral | .05mm Gd |
| $CH_4$ (upstream) (90K) | 11.5 × 12.0 × 4.4 | 6.5mm Boral | .05mm Gd |
| Para-$H_2$(downstream) (20K) | 12 × 11 × 7.6 | 1mm Cd | None |
| 20K para-$H_2$ used in place of $CH_4$: | | | |
| 6cm thickness | 11.5 × 12.0 × 6 | 6.5mm Boral | .05mm Gd |
| 8cm thickness | 11.5 × 12.0 × 8 | 6.5mm Boral | .05mm Gd |
| 10cm thickness | 11.5 × 12.0 × 10 | 6.5mm Boral | .05mm Gd |

Table 3: Moderator parameters for the split target.

| **Material** | **Dimensions ($cm^3$)** | **Decoupler** | **Poison** |
|---|---|---|---|
| $H_2O$ (wing) | 10 × 10 × 5 | 6mm boral | .05mm Gd |
| $H_2$ (wing) | 10 × 10 × 10 | None | None |
| $H_2O$ (flux trap) | 12 × 12 × 5 | 6mm boral | .05mm Gd |
| $H_2$ (flux trap) | 12 × 12 × 10 | 1mm Cd | .05mm Gd |

with other LCS codes.

The moderator performance in this paper was characterized by an estimate of the outgoing neutron current at 1eV in a direction normal to the moderator surface. This quantity was derived from the surface current $J_{calc}$ in the energy range 1eV to 1.47eV and in an angular bin defined by

$$0.75 < \cos\theta \leq 1.0$$

where $\theta$ represents the direction of the neutron relative to a normal to the moderator surface.

In general the outgoing current $J(\theta)$ from a moderator conforms to the approximate relationship

$$J(\theta) = J(0)\cos^2\theta \tag{1}$$

On the basis of equation (1) it can be shown that the relationship between $J(0)$ and $J_{calc}$ is approximately

$$J_0 = 1.30 J_{calc}$$

Equation (1) can also be used to estimate the reduction in moderator performance when it is viewed at a significant angle to the normal. For example, if an instrument sees the moderator surface at an angle $\theta = 20°$ this will reduce the detected neutron intensity by a factor of $\cos^2 20° = 0.883$.

## 5. Results and conclusions

### *5.1 Conventional target*

The results of the calculation of 1eV leakages (in a direction orthogonal to the surface of the moderator) are shown in Table 4. An interesting aspect of these results is the relatively small difference between the performance of 'upstream' and 'downstream' moderators. On the current ISIS target, with a proton beam energy of 800 MeV (as compared with 1.334 GeV for these calculations), the performance of the downstream moderators is worse than that of the upstream moderators by about a factor of two. It should be noted that our result is dependent on the placement of the moderators relative to the position of peak neutron 'brightness' from the target. In the ISIS target (proton energy 800 MeV) the front moderators coincide with the peak. The higher proton energy in our calculations shifts the peak further down the target so that it lies between the front and rear moderators, equalizing their performance. However, the positioning of moderators on the current ESS tantalum target (as modelled in [1]) is similar to ISIS; the front moderators are placed at the peak in neutron production, and the rear moderators again give a performance which is worse by about a factor of two.

Figs. 4 and 5 show the calculated leakage spectra below 1 eV for the methane moderator and the three replacement hydrogen moderators. The spectra were tallied in equal-lethargy energy groups, with six groups per decade.

The results indicate that a disadvantage of the hydrogen moderator would be a relatively poor performance in the energy range 20 to 100 meV; in the worst energy group the leakage from hydrogen is lower from methane by about a factor of two.

Table 4: Calculated 1 eV fluxes from the conventional target. The quantity $J(0)_{1eV}$ represents the neutron current at 1 eV per Sr per eV per cm$^2$ per second. The beam power of 1 MW represents a proton current of 750$\mu$A or 4.68 x $10^{15}$ protons per second.

| Moderator | $J(0)_{1eV}$ |
|---|---|
| $H_2O$ (upstream) | 2.77 x $10^{11}$ $\pm$ 2.3% |
| $H_2O$ (downstream) | 2.33 x $10^{11}$ $\pm$ 3.5% |
| $CH_4$ (upstream) | 2.42 x $10^{11}$ $\pm$ 0.8% |
| $H_2$ (downstream) | 2.78 x $10^{11}$ $\pm$ 3.3% |
| Replacement $H_2$ upstream moderators: | |
| 6cm | 2.24 x $10^{11}$ $\pm$ 1.3% |
| 8cm | 2.33 x $10^{11}$ $\pm$ 1.3% |
| 10cm | 2.50 x $10^{11}$ $\pm$ 1.2% |

Figs. 6 to 8 show examples of the calculated thermal time distributions for the methane and hydrogen moderators. The upper energy limit (indicated by a vertical dotted line in Figs. 4 and 5) was 46.5 eV for liquid methane or 21.5 eV for liquid hydrogen.

Table 5 shows calculated pulse width parameters for the four alternative moderators. Here the quantity $\Delta t_n$ represents the full width of the pulse at $n$% of its peak height [6]. Thus $\Delta t_{50}$ represents the full width at half maximum (FWHM); the other $\Delta t_n$ values indicate how rapidly the leakage intensity decays at later times.

The results indicate that an 8cm thick hydrogen moderator would produce a similar thermal time distribution to the 4.4cm methane moderator. The choice of an optimum thickness for the hydrogen moderator would be a compromise between the requirements of high neutron leakage and short time distributions. On the basis of these results, a thickness of about 8cm would be a reasonable choice. However, further optimization of a hydrogen moderator would probably be possible, e.g. by the use of a somewhat thicker moderator with two decoupler foils.

The anomalous thermal spectrum seen for the hydrogen moderator, with its strange peak at about 4 meV, is in conflict with measured spectra whose shape conforms more closely to a Maxwellian. It is believed that this result arises from the use of pure para-hydrogen in the model. A small proportion of ortho-hydrogen is probably be present in practice, and would significantly increase the total cross section at low energies.

Fig. 9 presents the results of a preliminary calculation to investigate the effect of a small proportion of ortho-hydrogen in the moderator. The spectrum from an 8cm liquid hydrogen moderator with with 5% ortho-, 95% para-hydrogen is compared with the spectrum previously calculated for a pure para-hydrogen moderator. The presence of the ortho-hydrogen changes the thermal spectrum significantly, removing the anomalous peak.

Table 5: Calculated pulse width parameters (in $\mu$s) for alternative poisoned methane and hydrogen moderators.

| Moderator | $\Delta t_{50}$ | $\Delta t_{30}$ | $\Delta t_{10}$ | $\Delta t_3$ | $\Delta t_1$ |
|---|---|---|---|---|---|
| Methane (4.4cm) | 26 | 43 | 79 | 126 | 175 |
| Hydrogen (6cm) | 24 | 34 | 57 | 93 | 146 |
| Hydrogen (8cm) | 30 | 43 | 71 | 121 | 180 |
| Hydrogen (10cm) | 37 | 52 | 91 | 145 | 211 |

Table 6: Results of moderator performance calculations. The quantity $J(0)_{1\text{eV}}$ represents the neutron current at 1eV per Sr per eV per cm$^2$ per second. The beam power of 1MW represents a proton current of 750$\mu$A or 4.68 $\times$ 10$^{15}$ protons per second.

| **Target dia. $D_T$(cm)** | 10 | 10 | 12 | 14 | 16 |
|---|---|---|---|---|---|
| **Beam dia. $D_B$(cm)** | 9 | 6 | 8 | 10 | 12 |
| **Beam Profile** | Gaussian (3$\sigma$ cutoff) | Parabolic | Parabolic | Parabolic | Parabolic |
| **Moderator** | **$J(0)_{1\text{eV}}(\times 10^{11})$** | | | | |
| $H_2O$ (flux trap) | 2.09 ± 1.8% | 2.16 ± 1.8% | 2.10 ± 1.8% | 1.91 ± 1.8% | 1.80 ± 2.0% |
| $H_2$ (flux trap) | 2.38 ± 1.9% | 2.46 ± 2.0% | 2.26 ± 2.0% | 2.25 ± 2.0% | 2.02 ± 2.1% |
| $H_2O$ (wing) | 2.28 ± 1.5% | 2.36 ± 1.4% | 2.10 ± 1.5% | 1.89 ± 1.6% | 1.72 ± 1.6% |
| $H_2$ (wing, no poison/decoupler) | 3.20 ± 1.4% | 3.19 ± 1.3% | 2.90 ± 1.4% | 2.59 ± 1.4% | 2.31 ± 1.6% |

*5.2 Split target*

The results of the calculation for $J(0)_{1\text{eV}}$ are given in Table 6. The results for the cases with a parabolic beam profile are presented in Figs. 10 and 11, in the form of plots of $J(0)_{1\text{eV}}$ vs. target diameter $D_T$. Figs. 10 and 11 show the results for flux trap and wing moderators, respectively.

The following conclusions can be drawn from the results:

1. The results in Table 6 indicate that the moderator performance is insensitive to the precise choice of beam profile. Here the change in $J(0)_{1\text{eV}}$ when the Gaussian profile is used in place of the parabolic profile is not statistically significant.

2. An optimum moderator configuration should probably match the performance of moderators in different locations. The chosen target-moderator configuration achieves this: the 'wing' moderators placed above and below the front section of the target give a similar performance to the

corresponding flux trap moderators.

3. A comparison of the plots in Fig. 10 and Fig. 11 reveals an interesting result: the performance of flux trap moderators is much less sensitive to target diameter than the performance of wing moderators.

4. A direct comparison between the two targets is possible for the two water moderators on the 10cm targets.

A comparison of the 'upstream' (front) water moderators on the two targets favours the conventional design. (See Tables 4 and 6. This moderator gives $J(0)_{1eV} = 2.77 \times 10^{11}$ neutrons cm$^{-2}$ eV$^{-1}$ Sr$^{-1}$ on the conventional target, compared with $2.28 \times 10^{11}$ on the comparable split target (about 80% of the performance on the conventional target.) In the case of the 'downstream' water moderator the results are more similar: $2.33 \times 10^{11}$ for the conventional target and $2.09 \times 10^{11}$ for the split target (about 90% of the performance on the conventional target.) Some caution must be exercised in interpreting this result, because no attempt has been made to arrive at a fully optimized configuration for the split target. However, it appears that the split target, as modelled for this paper, offers no advantage over a conventional target. This conclusion might be modified if the target diameter had to be increased substantially above 10cm. As indicated by Figs. Fig. 10 and Fig. 11, the consequent reduction in moderator performance would be significantly less for flux trap moderators than for wing moderators.

## 6. Acknowledgements

L.L. Daemen (Los Alamos National Laboratory) is acknowledged for the provision of geometry and materials specifications for the ISIS target.

## 7. References

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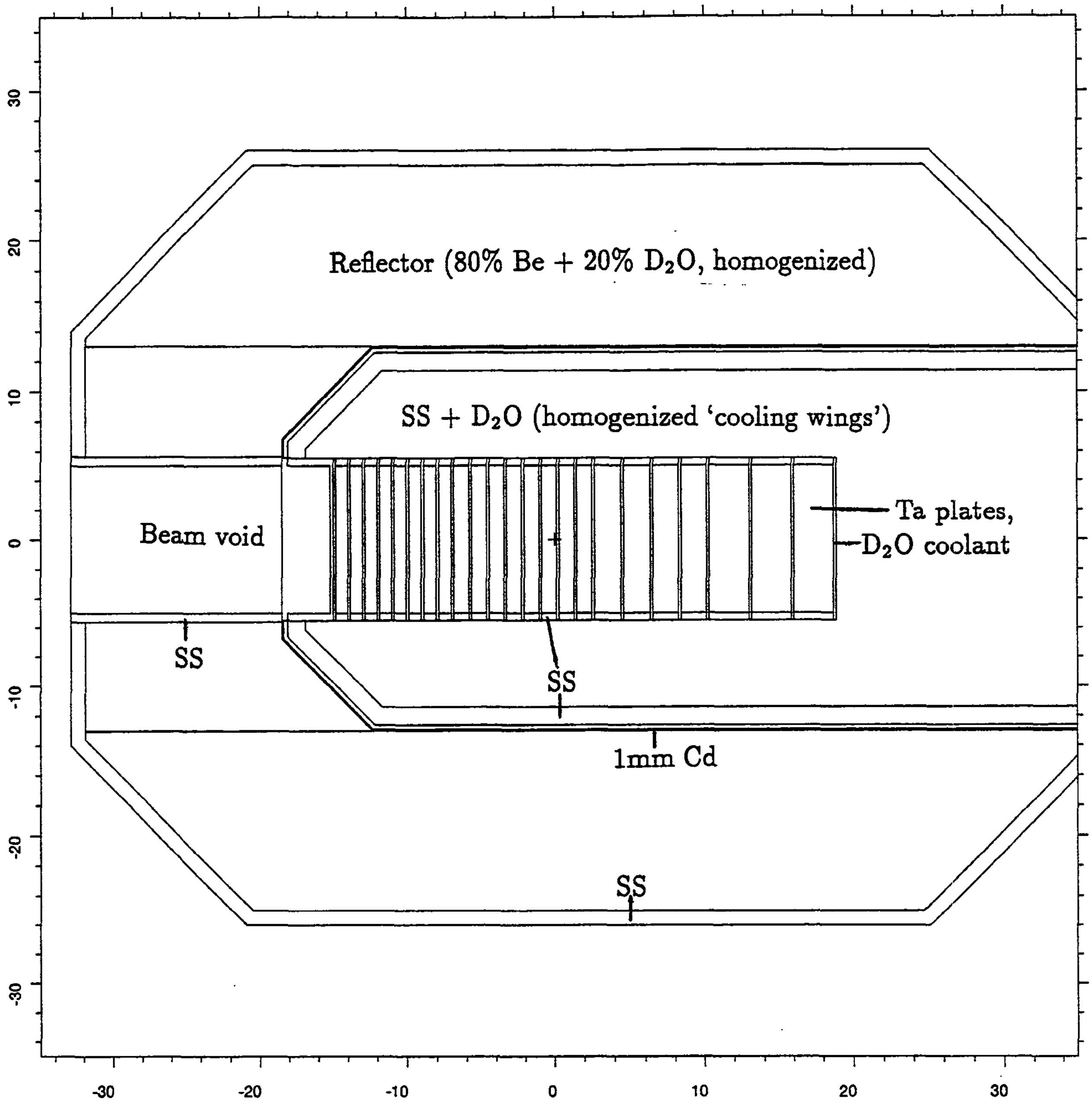


Fig. 1. Horizontal section through the conventional target showing the major components of the target-reflector assembly.

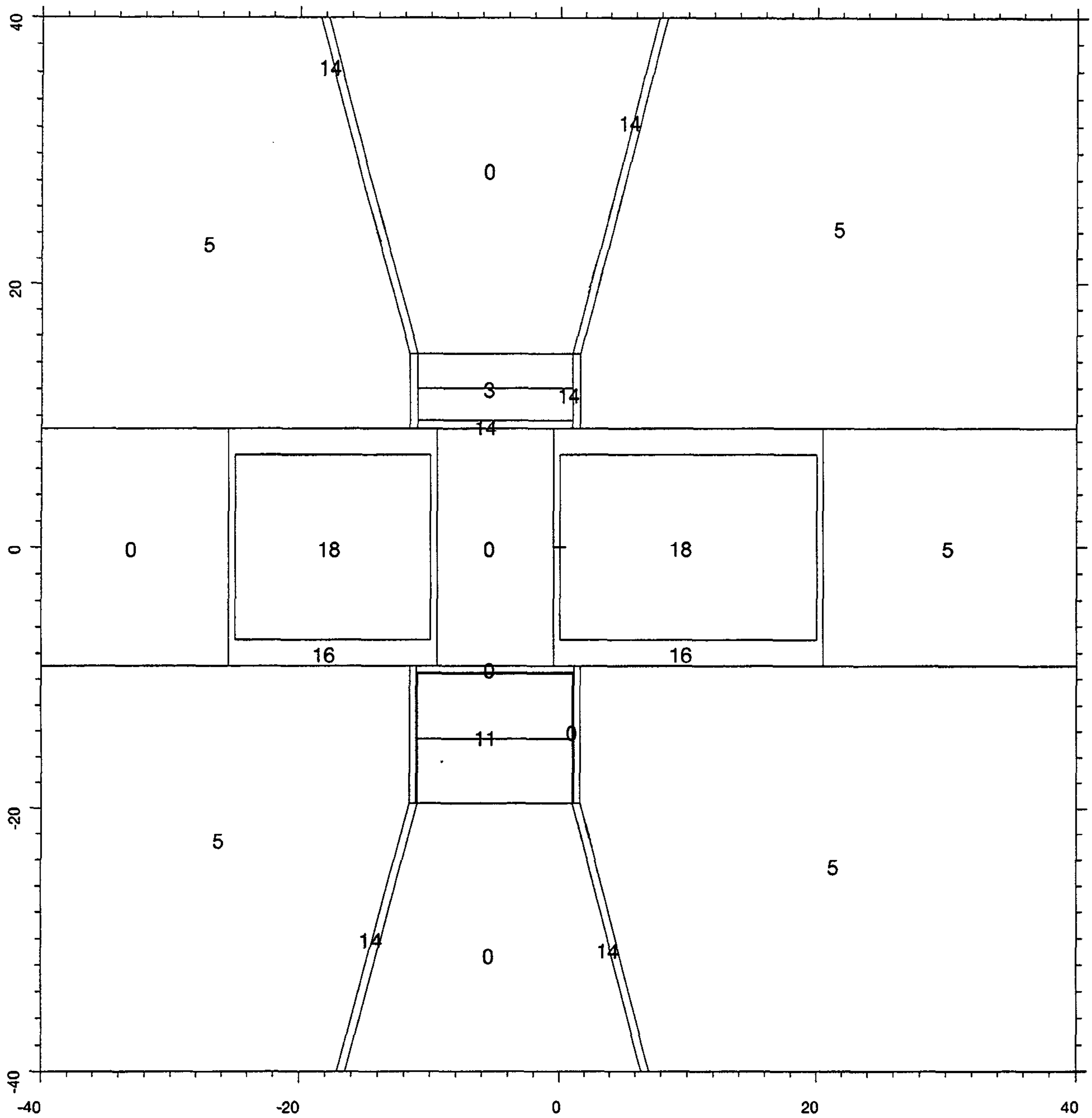


Fig. 2. Horizontal section through the split target geometry showing the front (left) and rear (right) target sections and the two flux trap moderators. The material numbers are listed in Table 1.

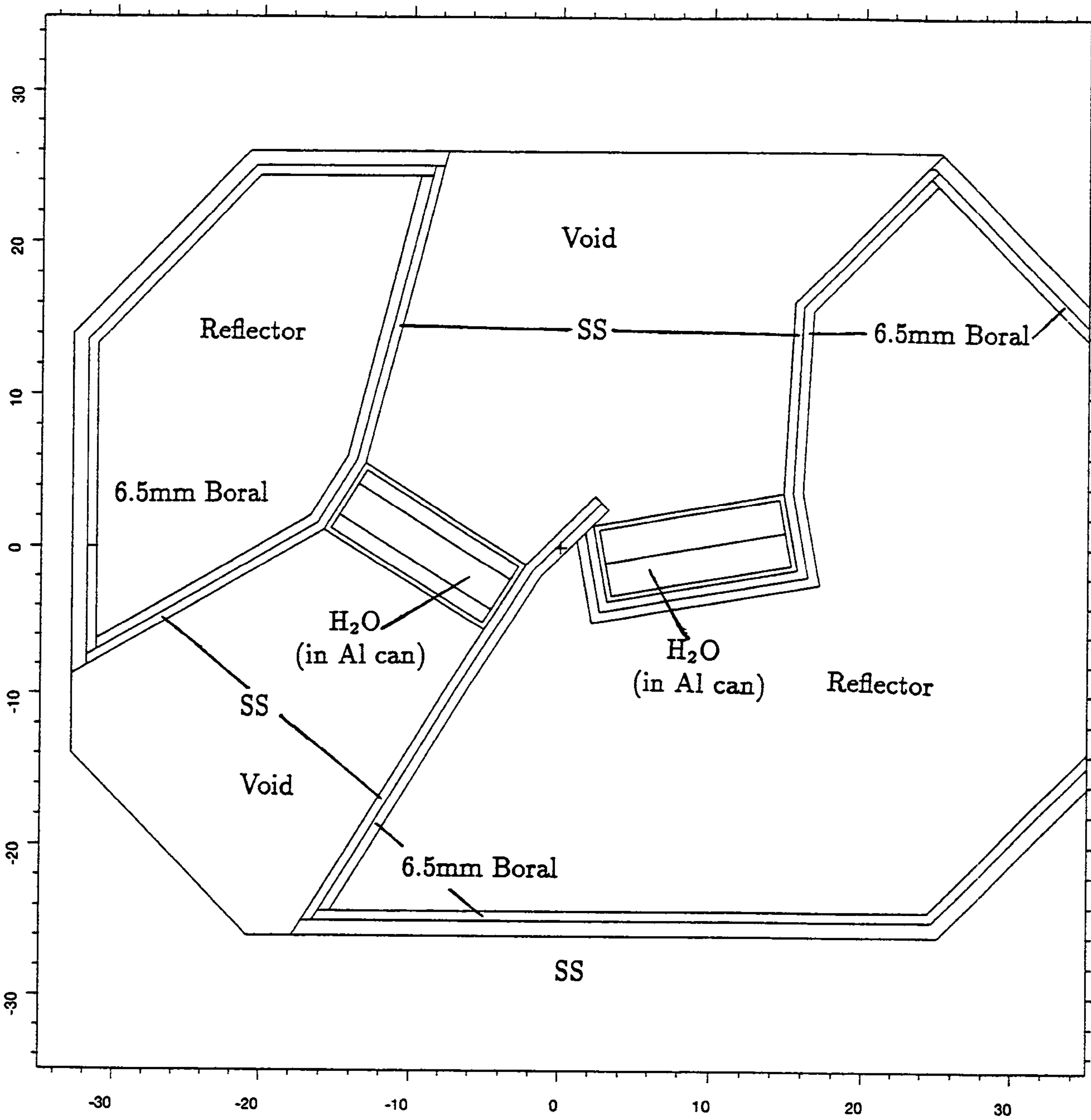


Fig. 3. Horizontal section through the upper (ambient temperature) moderators on the conventional target.

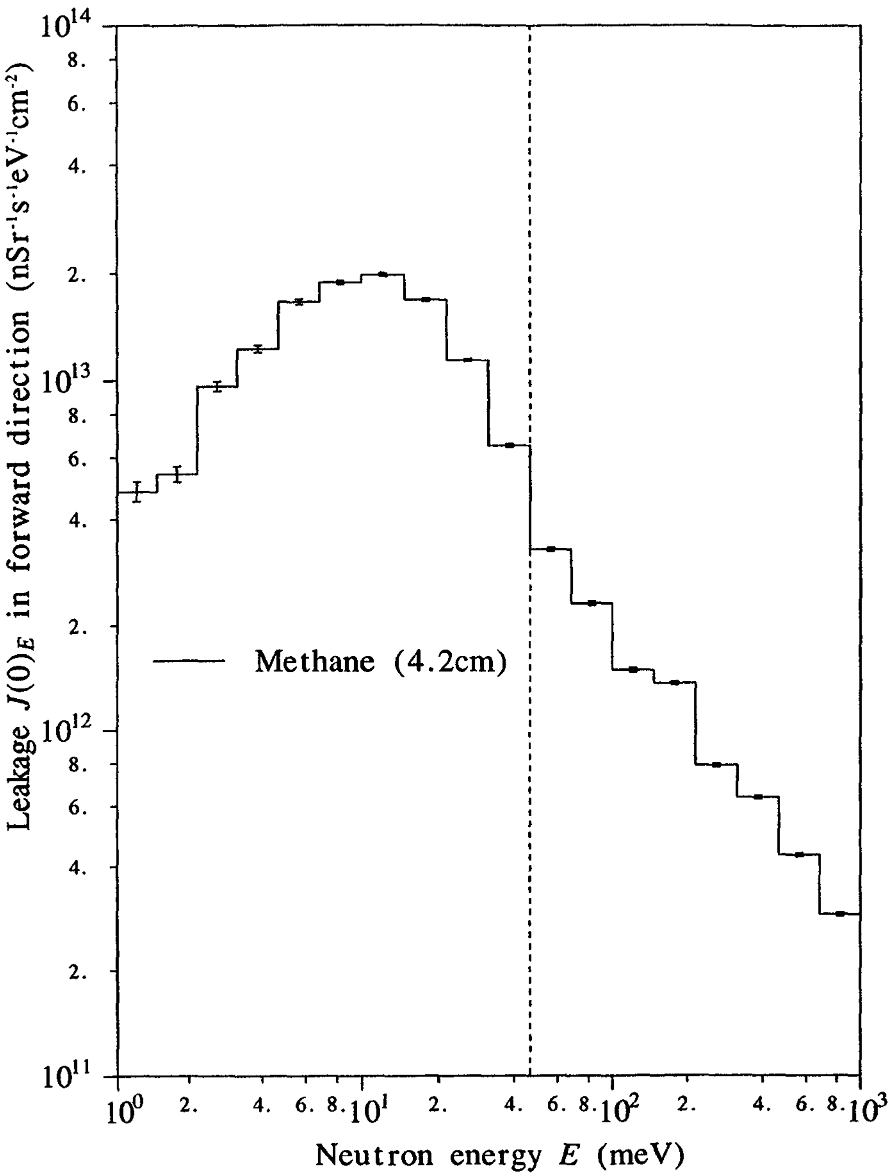


Fig. 4. Calculated leakage spectrum below 1eV from the 'upstream' methane moderator on the conventional target. The horizontal dashed line indicates the upper energy limit used for the calculation of thermal time distributions.

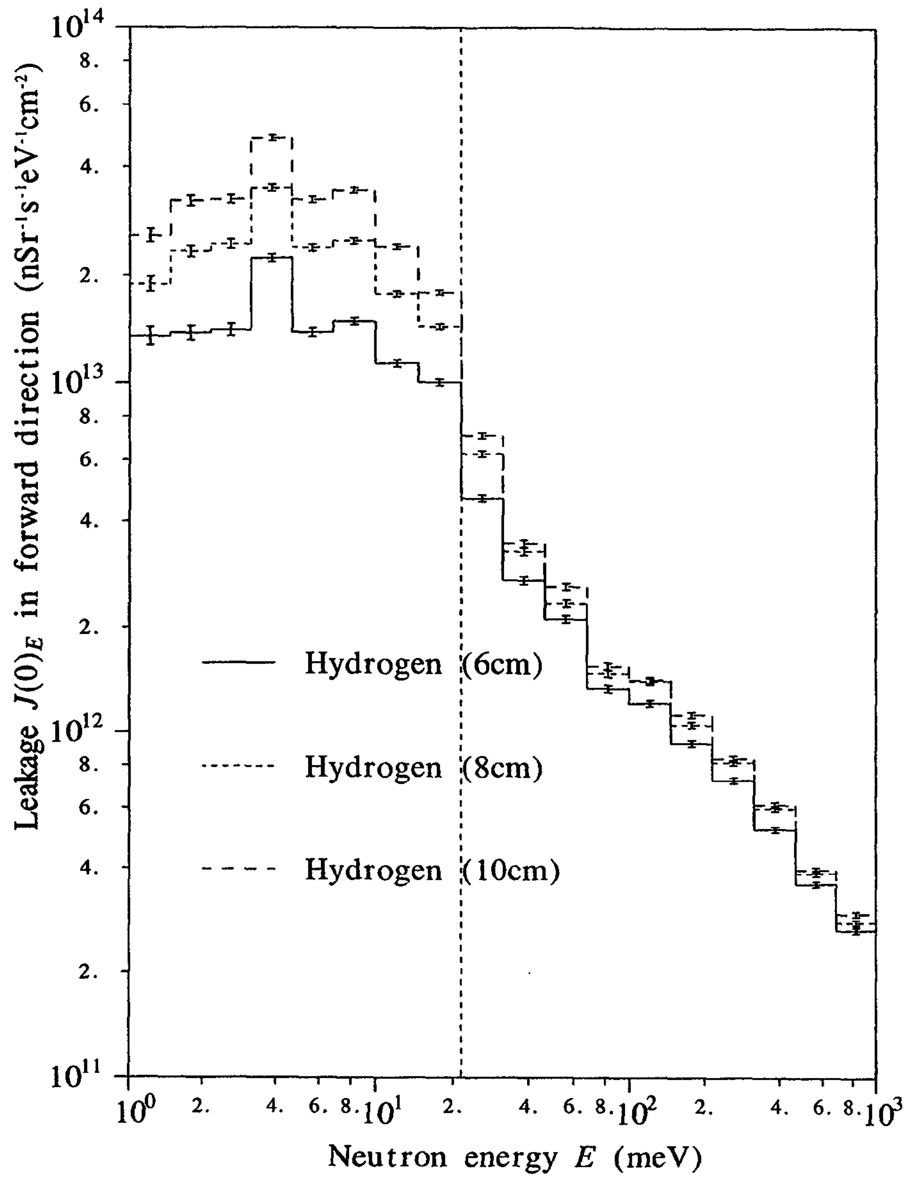


Fig. 5. Calculated leakage spectra from liquid hydrogen moderators used in place of the upstream methane moderator on the conventional target. The horizontal dashed line indicates the upper energy limit used for the calculation of thermal time distributions.

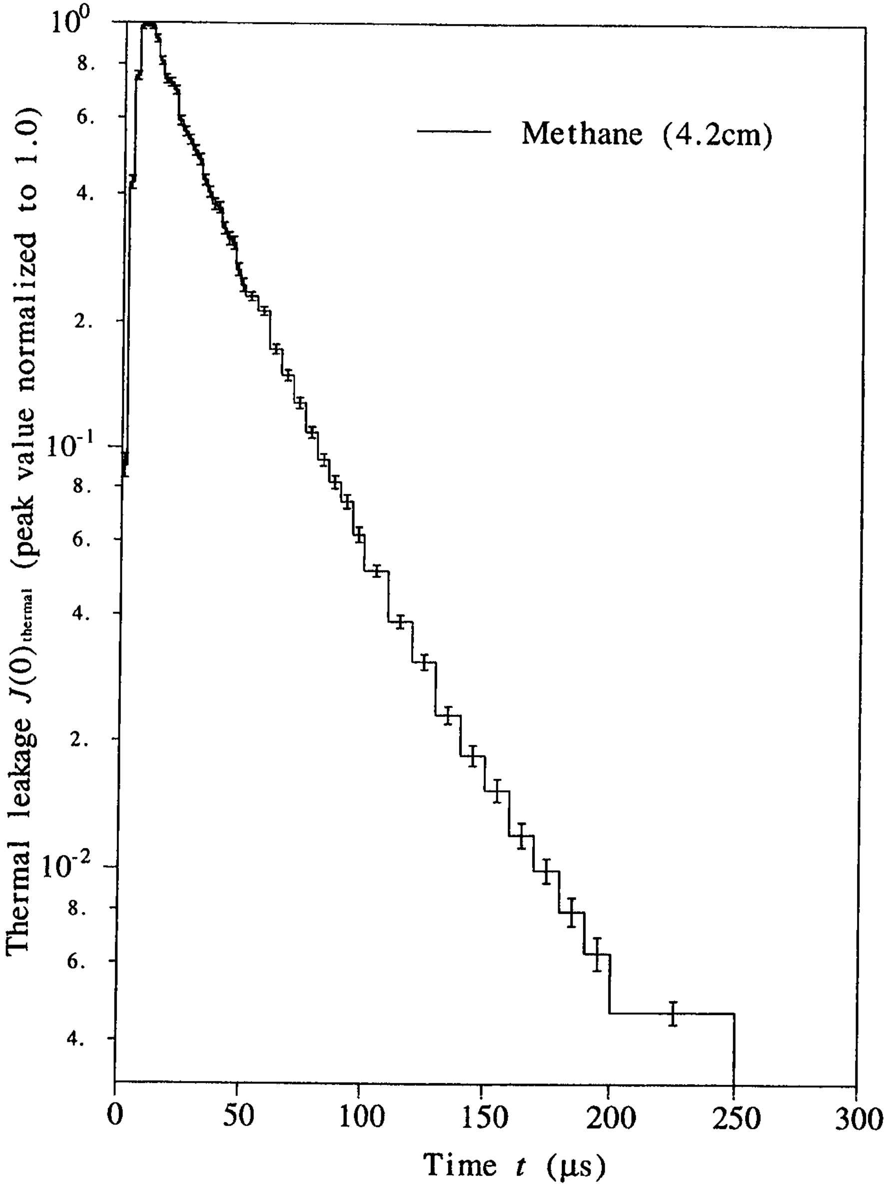


Fig. 6. Calculated thermal time distribution for the methane moderator on the conventional target.

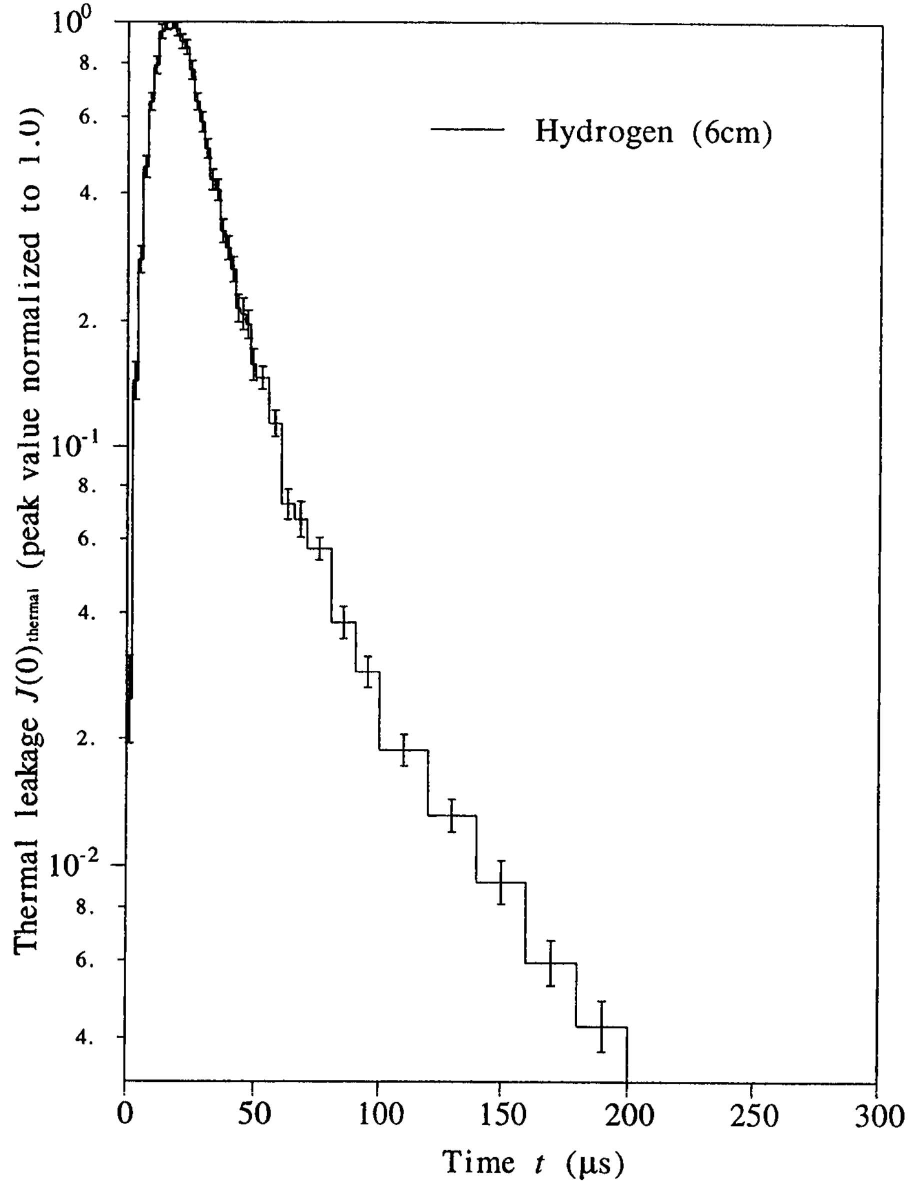


Fig. 7. Calculated thermal time distribution for the 6cm hydrogen moderator used in place of the methane moderator on the conventional target.

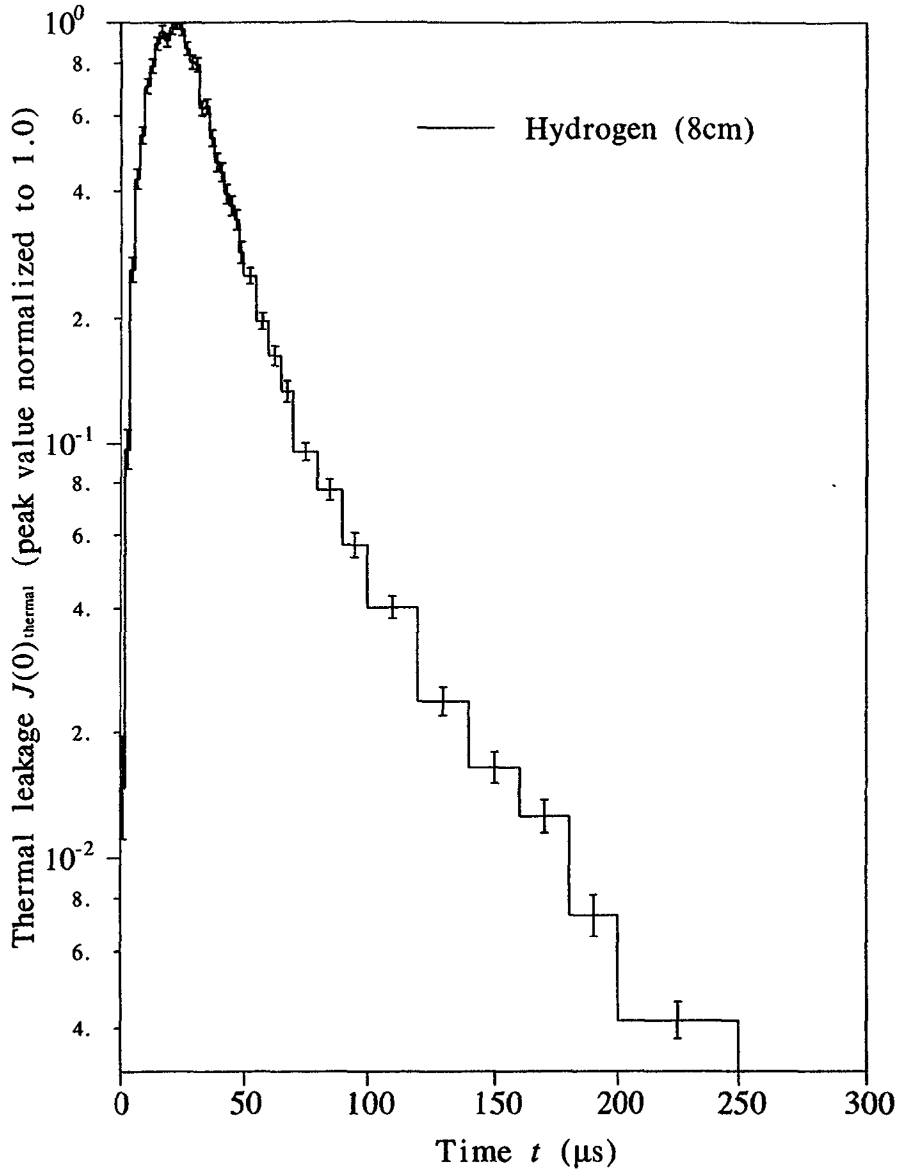


Fig. 8. Calculated thermal time distribution for the 8cm hydrogen moderator used in place of the methane moderator on the conventional target.

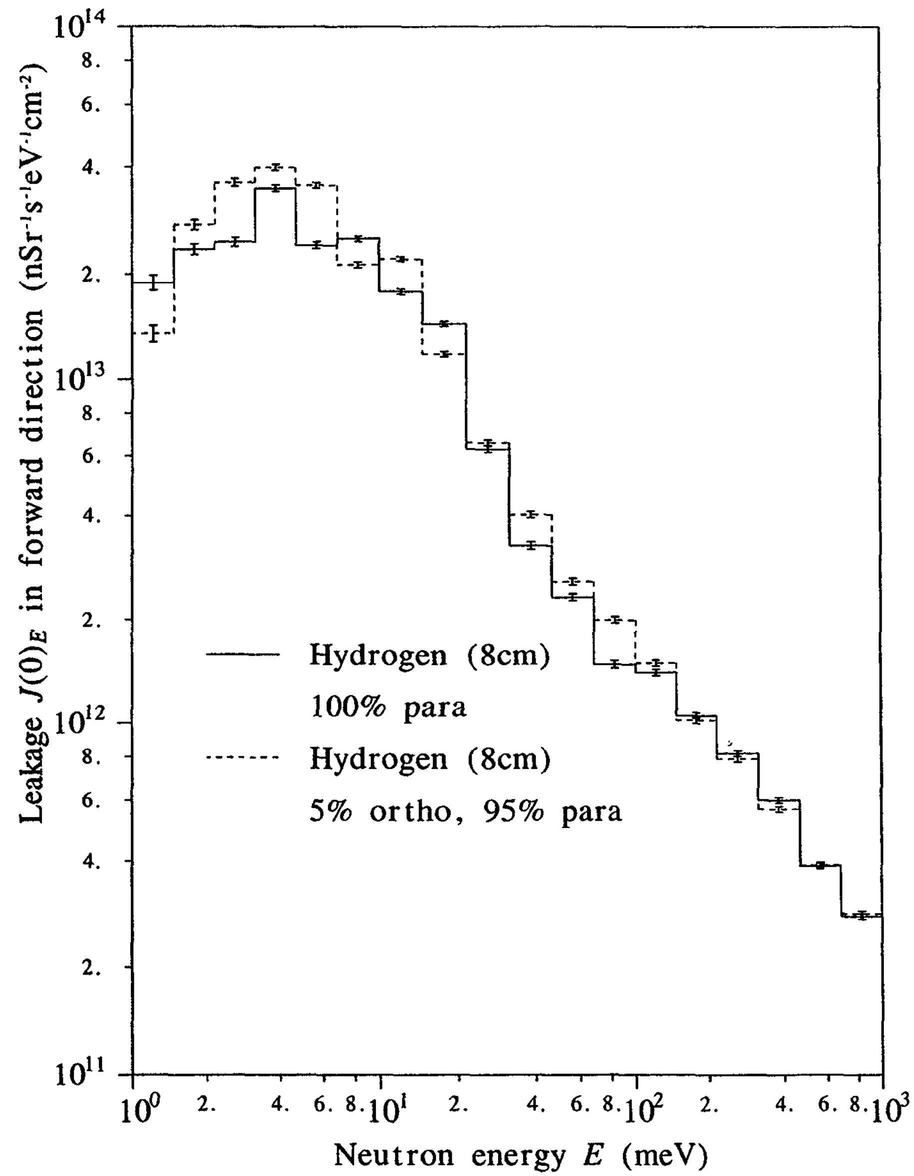


Fig. 9. Comparison of calculated neutron spectra from pure para-hydrogen (8cm) and 5% ortho-, 95% para-hydrogen (8cm).

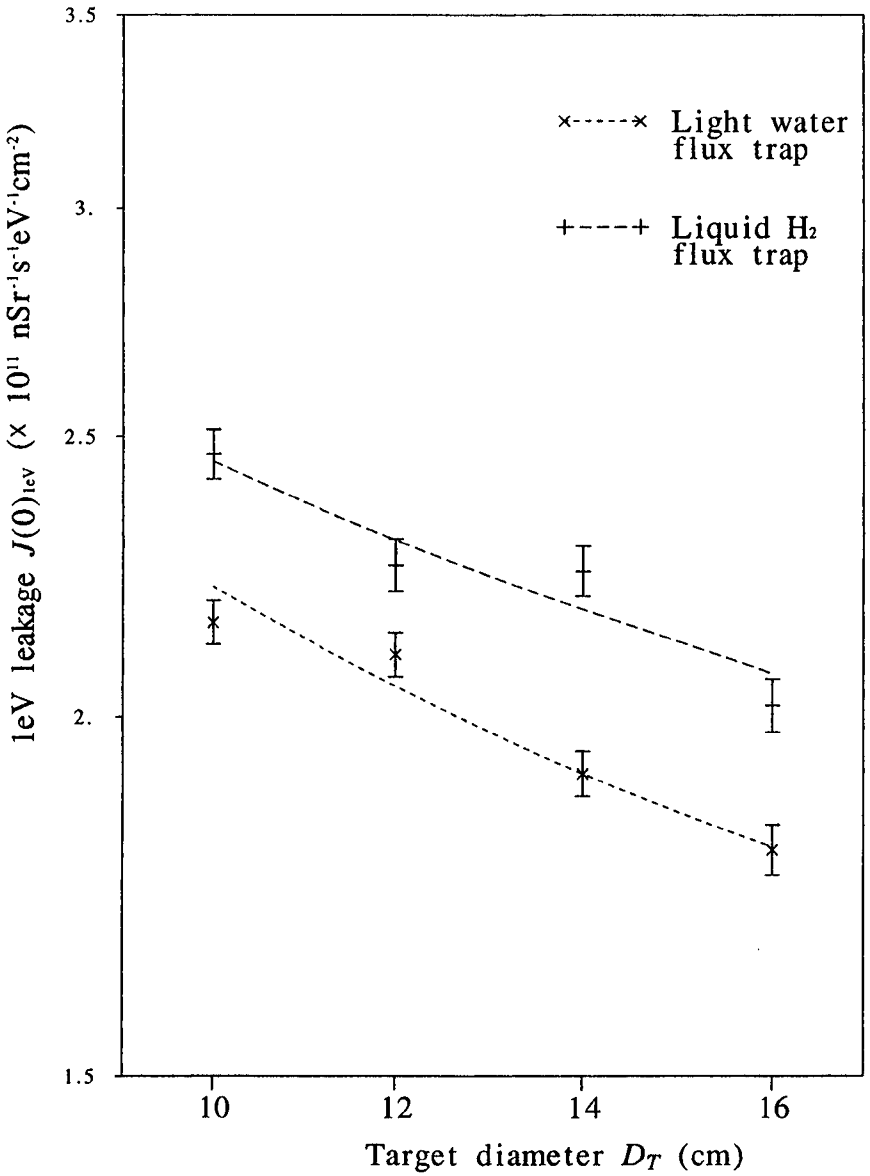


Fig. 10. Performance of the flux trap moderators on the split target (characterized by the 1eV leakage) as a function of target radius.

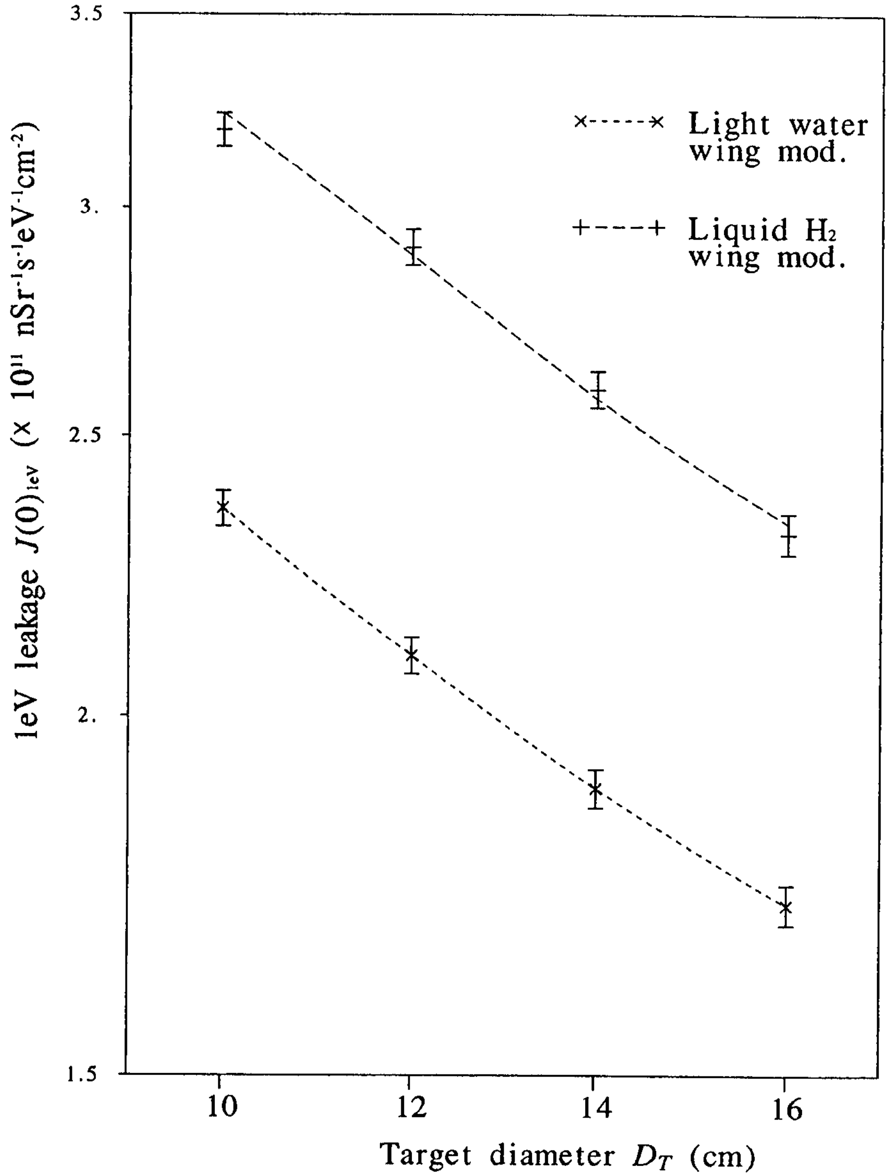


Fig. 11. Performance of the wing moderators on the split target (characterized by the 1eV leakage) as a function of target radius.