Design of neutron moderators for ESS

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for the ESS neutronics team

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Our way to the butterfly
Outline

1. European Spallation Source
2. Flat moderators
3. Butterfly
4. Instruments
5. Conclusions
### Nomenclature

**Neutron energy range**

<table>
<thead>
<tr>
<th>Cold</th>
<th>Thermal</th>
</tr>
</thead>
<tbody>
<tr>
<td>$&lt;$ 5 meV</td>
<td>20 – 100 meV</td>
</tr>
<tr>
<td>$&gt;$ 4 Å</td>
<td>0.9 – 2 Å</td>
</tr>
</tbody>
</table>
Several intra-nuclear cascade (INC) models (Bertini, Isabel, INCL4) and evaporation/fission models (Dresner, ABLA), as well as the self-contained package CEM03, were employed for simulation of high-energy physics in MCNPX. The results are shown in Figure 3.13 (top left). Apart from the INCL4 INC model, the models returned values within $\pm 5\%$ of each other for neutronic performance and heat deposition. The intermediate energy region (above a few eV) is especially important for the neutronics of moderators and reflectors. Three neutron libraries, ENDF/B-VII.0 (US), JENDL-4.0 (Japan), and JEFF3.1 (Europe), were tested on system components, with the results shown in Figure 3.13 (top right). The differences in neutronic performance was again found to be within $\pm 5\%$. Neutron scattering kernels are used for detailed simulation of neutron transport at thermal energies and below. Figure 3.13 (bottom left) shows that the use of scattering kernels at ambient temperatures is not crucial: the difference between free gas treatment and $(\alpha,\beta)$ formalism is within 5% for non-cryogenic parts. Scattering kernels are, however, absolutely necessary for cryogenic parts, for example, liquid hydrogen. The difference in neutronic performance and heat deposition due to the difference in para-hydrogen scattering kernels is illustrated in Figure 3.13 (bottom right).

The analysis shows that uncertainties associated with nuclear interaction models and nuclear data libraries are expected to be about 15%. While almost any combination of models and libraries studied would suffice (with the notable exception of the outdated MCNPX INCL4 INC model), the default MCNPX Bertini-Dresner model coupled with ENDF/B-VII.0-based neutron libraries and scattering kernels (when-22ever available) are recommended to simplify inter-comparison of neutronic results. The default MCNPX nuclear interaction model is generally accepted by the spallation source community for calculating most quantities of interest, such as neutronic performance and nuclear heating [334]. In addition, it requires less computing time than other models and is therefore preferred for optimisation studies.

### 3.2.4 Optimisation of the beam-target interface

Optimisations of the neutronic design were performed by choosing integral values of the cold or thermal neutron brightness as the figure of merit:

$$\text{FoM} = \int_0^\infty dt \int_{E_c}^0 \Phi(t,E)dE$$

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**Volume**

- Thermal moderator ($\text{H}_2\text{O}$)
- $\sim 16 \times 16 \times 13 \text{ cm}^3$

**Butterfly**

- $\sim 20 \times 30 \times 3 \text{ cm}^3$
European Spallation Source (ESS)

- Lund, Sweden
- First neutrons by 2019

http://europeanspallationsource.se
European Spallation Source (ESS)

- Proton beam:
  - $2 \text{ GeV} \times 2.5 \text{ mA} = 5 \text{ MW}$
  - $14 \text{ Hz, 2.86 msec}$

- Tungsten rotating target

- Cold neutrons:
  - Para-$\text{H}_2$ at 20 K

- Thermal neutrons:
  - Water at 300 K
1 European Spallation Source
2 Flat moderators
3 Butterfly
4 Instruments
5 Conclusions
Starting point: baseline configuration
J-PARC style cold moderator

- Para-$H_2$ volume moderator 13 cm high $\times$ 8 cm radius
- Thermal wings provide a bi-spectral source
Starting point: baseline configuration
J-PARC style cold moderator

F. Maekawa et al
First neutron production utilizing J-PARC pulsed spallation neutron source JSNS and neutronic performance demonstrated (2010)
Excellent performance from the volume moderators

- Cold: ×60 ILL Yellow Book
- Thermal: ×7 ILL Yellow Book
- × 2 ESS 2003

[ESS Technical design report, page 178]
How to make it better?

- Planned 1 year time to improve the moderator design
Optimisation
Cylindrical moderator dimensions
Unperturbed brightness
Cylindrical moderator performance as a function of its dimensions

Moderator size for highest cold brightness: ø = 15 cm h = 1.4 cm
Unperturbed brightness
Cylindrical moderator performance as a function of its dimensions

Moderator size for highest cold brightness:
\[ \varnothing = 15 \text{ cm} \quad h = 1.4 \text{ cm} \leftarrow \text{Pancake} \]
Unperturbed brightness
Cylindrical moderator performance as a function of its dimensions

Moderator size for highest cold brightness:
\[ \varnothing = 15 \text{ cm} \quad h = 1.4 \text{ cm} \leftarrow \text{Pancake} \]

[K. Batkov et al, 2013]
Why flat moderators work
Cold neutron map in volume moderator

- Neutrons are effectively moderated within 1 – 2 cm of liquid hydrogen
Why flat moderators work
Cold neutron map in volume moderator

[Image of a graph showing the brightness in n/cm²/sec/sr as a function of distance to the target centre in cm. The graph is color-coded with a legend indicating the range from 0 to 10^13.]
Why flat moderators work
Cold neutron map in volume moderator

- Behaviour used and measured at J-PARC

T. Kai, M. Harada, M. Teshigawara, N. Watanabe, Y. Ikeda
Coupled hydrogen moderator optimization with ortho/para hydrogen ratio
2004
Why flat moderators work
Cold neutron maps in volume and flat moderators

**Volume moderator**

- **Reflector side**
- **Target side**

**Flat moderator**

- **Target side**

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**Distance to the target centre [cm]**

**Brightness [n/cm²/sec/sr]**

- **Flat**
- **Volume**

- \(10^{13}\)
Why flat moderators work
Angular distribution

Flat moderator shows a strong effect at small vertical emission angles

[K. Batkov et al, 2013]
Properties of para-$\text{H}_2$

Scattering cross-section

- Significant drop of $\sigma$ below 50 meV ⇒
- Medium is almost transparent for cold neutrons

$\sigma_{\text{total}}$ [barn]

Energy [eV]

T=20 K

[New para-$\text{H}_2$ data]

[N. Watanabe, Neutronics of pulsed spallation sources, 2003]
Mean free path below 50 meV becomes comparable to the height of the small optimised moderator, making the whole volume to be the source of neutrons.
Why flat moderators work
Perturbation effect

- Less reflector material is removed in the case of flat moderator ⇒
- No difference between openings $2 \times 60^\circ$ and $2 \times 120^\circ$ ⇒
- Possible to serve more instruments
Importance of pure para-$\text{H}_2$

- Extreme dependency of the brightness on the purity of para-$\text{H}_2$
- Importance of the catalyst
- More than 99% para measured at J-PARC
- Experimental measurements at high power required
Moderator should be as tall as needed by instruments

At 3 cm 80% of total neutrons emitted compared to maximum
Why flat moderators work

Physics summary

■ Neutrons are **effectively moderated within 1-2 cm** of para Hydrogen

■ Para-hydrogen transparency window allows to collect neutrons from depth

■ With respect to volume moderators:
  ■ **Less parasitic absorption** due to smaller amount of Hydrogen (with respect to volume moderators)
  ■ **Less perturbation** due to smaller amount of reflector removed

■ However: very sensitive to **para-H₂ purity**
Butterfly moderator
Para-H$_2$
Butterfly moderator
Para-H₂ and water
Butterfly moderator
Horizontal cut
Butterfly moderator
Target wheel and Moderators

R=1.25 m
3 cm
6 cm

[Bengt Jönsson]
Butterfly moderator
Target wheel and Moderators: vertical cut

Protons
Butterfly moderator
Horizontal view

Protons 2 meters
Butterfly moderator
Cold neutron extraction
Butterfly moderator
Cold neutron extraction

![Graph showing cold neutron brightness as a function of instrument location.]

Cold brightness $[\text{n/cm}^2/\text{sec/sr}]$

- $10^{13}$

Instrument location $[\text{deg}]$

-60  -40  -20  0  20  40  60

Statistical errors $\sim 1\%$

[Esben Klinkby, TAC11, page 17]
Butterfly moderator
Thermal neutron extraction
Butterfly moderator
Thermal neutron extraction

Thermal brightness [n/cm²/sec/sr]

-60 -40 -20 0 20 40 60

Instrument location [deg]

-60 -40 -20 0 20 40 60

Thermal brightness [n/cm²/sec/sr]

3 cm

6 cm

Statistical errors ~ 1 %

[Esben Klinkby, TAC11, page 17]
Optimisation of Instrument Suite
Example 1: NMX — macromolecular diffractometer

Data provided by Ken Andersen, ESS
Optimisation of Instrument Suite
Example 1: NMX — macromolecular diffractometer

Data provided by Ken Andersen, ESS
Optimisation of Instrument Suite
Example 1: NMX — macromolecular diffractometer

Data provided by Ken Andersen, ESS
Example 2: ESSENSE — spin echo spectroscopy

Data provided by Ken Andersen, ESS
Optimisation of Instrument Suite
Optimal moderator height

Ken Andersen, Moderator/Instruments Meeting, 6 June 2014
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Wavelength spectra

Peak brightness [n/cm²/sec/sr/Å] vs Wavelength [Å]

- TDR cold
- TDR thermal

Statistical errors < 5 %
Wavelength spectra

Statistical errors < 5 %
Wavelength spectra

Wavelength [Å]

Peak brightness [n/cm²/sec/sr/Å]

- TDR cold
- TDR thermal
- Low butterfly cold
- Low butterfly thermal
- Top butterfly cold
- Top butterfly thermal

Statistical errors < 5%
Integrated brightness

Cold (< 20 meV) brightness [a.u.]

- Low butterfly 3 cm: 1.8
- Top butterfly 3 cm: 2.86
- TDR: 1
Integrated brightness

- **Low butterfly 3 cm**: 2.08
- **Top butterfly 3 cm**: 3.01
- **TDR**: 1

Thermal (20 – 100 meV) brightness [a.u.]
Two butterfly moderators, each serving $2 \times 120^\circ$ sector
- Upper: 3 cm tall
- Lower: 6 cm tall

Exploits all neutronic design criteria developed

Optimal beam extraction
- Flexible to place instruments
- Flexible for instruments to choose moderator
- Optimal for bispectral instruments

Feasible engineering
References

F. Mezei, L. Zanini, A. Takibayev, K. Batkov, E. Klinkby, E. Pitcher, T. Schönfeldt,
Low dimensional neutron moderators for enhanced source brightness
arXiv:1311.2474
2013

K. Batkov, A. Takibayev, L. Zanini, F. Mezei
Unperturbed moderator brightness in pulsed neutron sources
Nuclear Instruments & Methods in Physics Research A
http://dx.doi.org/10.1016/j.nima.2013.07.031
2013
Thank you for your attention
FIG. 6. (Color online) Total cross section from this work in b/atom (triangles); parahydrogen scattering cross section (squares). The upper error bar on the parahydrogen cross section comes from Table I and the lower error bar is given by the upper limit on the orthohydrogen contamination.