SIMULATING NEUTRON TRACKS IN THE NEW TS1-TRAM AT ISIS WITH FLUKA CODE: SOME INSIGHTS TOWARDS AN OPTIMISED AND MORE EFFICIENT TARGET-MODERATOR-REFLECTOR ASSEMBLY FOR HIGH POWER SPALLATION SOURCES

L. Quintieri, S. Lilley
OUTLINE

• The FLUKA model of the upgraded ISIS-TS1 TRAM
  ❖ A general overview

• “Standard” simulation results (feedback on accuracy of the model):
  ❖ Fluence spectra of escaping particles (not only neutrons)
  ❖ Energy deposition comparison with MCNP (indirect model validation)

• “Advanced” simulations for neutron tracking (for a more efficient TRAM design):
  ❖ Target plate contribution to the neutron TRAM leakage (i.e. neutron plate efficiency to improve the target design)
  ❖ “Flagging” neutrons across clue regions (i.e. moderators) to assess their effective contribution to the instrument beam (some specific estimation on Polaris and Maps)

• “Conclusion & ongoing activity”
ISIS: PULSED NEUTRON & MUON SPALLATION SOURCE

- ISIS is one of the world’s leading spallation neutron and muon facilities
- ISIS accelerators drive neutron and muon factory
- ~750 experiments/year
- ~1500 visitors/year (~4500 visits)

ISIS has more than 20 international partnerships and agreements with 11 different countries.

- Sweden: 5-year agreement with the Swedish Research Council from January 2015.
- India: A 5-year agreement with India to provide contributions to the Zoom instrument.
- Italy: Renewal of a 6-year agreement with Italy, contributing to several ISIS instruments.
- The Netherlands
- Japan
- China
- Spain
- USA
- UK

Rutherford Appleton Laboratory in Harwell Campus-Oxford

UKRI: STFC Science & Technology Facilities Council
**Targets**  
2 × W (Ta coated)

**Protons**  
800 MeV

- The ISIS accelerator produces a beam pulse at 50Hz with every fifth pulse delivered to TS-2, the rest to TS-1.

- Currently ISIS has two spallation targets, TS1 operating at proton beam powers of up to 200 kW, and TS2 operating to 45 kW.

**Number of Instruments**
- **TS1** 27 (20n+7µ)
- **TS2** 11

**Types of Instrument at ISIS**
- Diffractionometer
- Reflectometer
- Small Angle Scattering
- Indirect Spectrometer
- Direct Spectrometer
- Muon Spectrometer/Instrument
- Neutron Irradiation
- Imaging and Diffraction
FLUKA MODEL OF THE UPDATED TS1-TRAM
GEOMETRY, PHYSICS, SOURCE
TRAM MODULE: UPDATES

- Smaller Reflector: the SS vessel filled with Be rods changed with a Be multi brick structure, edge cooled
- Boral layer around the reflector
- Flight-line liners: steel removed, only Boral
- Cooling pads added

- Methane moderator: 3rd aluminum layer removed, Second Gd foil inserted
- Hydrogen moderator: height reduced
- Inserted water pre-moderators
- Target shape changed from rectangular to cylindrical
- 10 plates in place of 12

<table>
<thead>
<tr>
<th>Material</th>
<th>Current Ts1</th>
<th>TS1 Upgrade</th>
<th>Reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS</td>
<td>73.8</td>
<td>8.1</td>
<td>89%</td>
</tr>
<tr>
<td>Ta</td>
<td>32.7</td>
<td>6.9</td>
<td>79%</td>
</tr>
<tr>
<td>W</td>
<td>47.3</td>
<td>46.0</td>
<td>2.8%</td>
</tr>
<tr>
<td>Total</td>
<td>153.8</td>
<td>61.0</td>
<td>60.3%</td>
</tr>
</tbody>
</table>
UPGRADED TS1 TRAM: THE FLUKA MODEL

Detailed geometry
1683 regions and 31 materials cards used for the model

Post-process oriented model in order to get direct neutron track-length density estimation in each assemblies and subassemblies that could be "monitored" or "measured".
GEOMETRIC ACCURACY OF THE MODEL

The target core is made of 10 tungsten plates, each of 4.9 cm radius, cladded with tantalum (cladding thickness is 0.2 cm).

Ta cladded thermocouples are introduced in the Fluka model as well.

FIGURE OF MERIT: Very accurate model of the whole TRAM: between CAD and FLUKA model, the maximum difference in the volumes for each components is always less than 3%.
### Primary Beam Characteristics

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle</td>
<td>Protons</td>
</tr>
<tr>
<td>Energy profile</td>
<td>Gaussian</td>
</tr>
<tr>
<td>Mean Energy</td>
<td>800 MeV</td>
</tr>
<tr>
<td>Energy spread</td>
<td>±0.4%</td>
</tr>
<tr>
<td>FWHM</td>
<td>7.4 MeV</td>
</tr>
<tr>
<td>Spatial profile</td>
<td>Gaussian</td>
</tr>
<tr>
<td>FWHM</td>
<td>4.2 cm</td>
</tr>
<tr>
<td>Divergence in V</td>
<td>100 π mm-mrad</td>
</tr>
<tr>
<td>Divergence in H</td>
<td>90 π mm-mrad</td>
</tr>
<tr>
<td>Angular divergence</td>
<td>0.88 mrad</td>
</tr>
</tbody>
</table>

**Proton density (2D projections)**

**Proton density (1D projection)**
ENERGY DEPOSITION PROFILE:
COMPARISON WITH THE MCNP REFERENCE MODEL
Beam Power = 160 kW
Deposited power = 108 kW

Hydrogen moderator operates at 20K

<table>
<thead>
<tr>
<th>MATERIAL</th>
<th>FLUKA (MeV/pr)</th>
<th>MCNP** (MeV/pr)</th>
<th>Δ/MCNP</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Total</strong></td>
<td>541.5 ±0.4%</td>
<td>474.6</td>
<td>14%</td>
</tr>
<tr>
<td>Water</td>
<td>0.881 ±0.05</td>
<td>0.84</td>
<td>4.6%</td>
</tr>
<tr>
<td>Boral (decoupler)</td>
<td>2.042 ±4.68E-2</td>
<td>1.84</td>
<td>11%</td>
</tr>
<tr>
<td>Poison (Gd+Al)</td>
<td>0.017 ±5.6E-3</td>
<td>0.04</td>
<td>57%</td>
</tr>
</tbody>
</table>
ENERGY DEPOSITION: PARTICLE CONTRIBUTION

Rate of secondary escaping particles from TRAM (primary beam: 800 MeV proton - 200μA

<table>
<thead>
<tr>
<th>Source strength (s⁻¹)</th>
<th>Neutron (MeV/pr)</th>
<th>Proton (MeV/pr)</th>
<th>Pion +/-(MeV/pr)</th>
<th>Muon +/-(MeV/pr)</th>
<th>Photon (MeV/pr)</th>
<th>Electron (MeV/pr)</th>
<th>Positron (MeV/pr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total</td>
<td>7E+15</td>
<td>4E+13</td>
<td>1.8E+12</td>
<td>2.5E+11</td>
<td>1E+16</td>
<td>7E+13</td>
<td>6.5E+12</td>
</tr>
</tbody>
</table>

REFLECTOR

<table>
<thead>
<tr>
<th>REFLECTOR</th>
<th>FLUKA (MeV/pr)</th>
<th>MCNP (MeV/pr)</th>
<th>Δ/</th>
<th>MCNP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total</td>
<td>82.86 ± 7%</td>
<td>80.77</td>
<td>3%</td>
<td></td>
</tr>
<tr>
<td>Be</td>
<td>54.24</td>
<td>58.97</td>
<td>8%</td>
<td></td>
</tr>
</tbody>
</table>

E_{dep} (MeV/pr)

<table>
<thead>
<tr>
<th></th>
<th>TRAM</th>
<th>TARGET</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total</td>
<td>541.5 ± 2.3%</td>
<td>427</td>
</tr>
<tr>
<td>Neutron</td>
<td>37</td>
<td>4.2</td>
</tr>
<tr>
<td>Proton</td>
<td>401</td>
<td>380</td>
</tr>
<tr>
<td>Gamma</td>
<td>1.6</td>
<td>1.5</td>
</tr>
</tbody>
</table>
NEUTRON YIELD
**NEUTRON BALANCE IN THE WHOLE TRAM**

**Bare target:**
- An average of **14.1 neutrons** per impinging 800 MeV proton **escaping from the target**.
- **83.5%** of the escaping neutrons are produced in **Tungsten**

**TRAM:**
- An average of **5.3 neutrons** per impinging 800 MeV proton **escaping from the TRAM**.
- **68%** of the escaping neutrons are produced in **Tungsten**

**NIM 145 (1977) 91–13 JM Carpenter**

NEUTRON BALANCE IN THE WHOLE TRAM

** NIM 145 (1977) 91-13 JM Carpenter

- An average of **14.1 neutrons** per impinging 800 MeV proton *escaping from the target*.
- **83.5%** of the escaping neutrons are produced in **Tungsten**

** TRAM:**
- An average of **5.3 neutrons** per impinging 800 MeV proton *escaping from the TRAM*.
- **68%** of the escaping neutrons are produced in **Tungsten**
More than 2/3 of the target produced neutrons is lost, taking into account that also the auxiliary materials (i.e. Beryllium, etc) are contributing.

2 possible options to increase the neutrons flux have been investigated so far:

- **Option1**: Increasing the primary proton energy. This implies the increasing of the neutron rate over all the energy spectrum (i.e. not optimised for useful neutrons only) and more severe energy deposition issues.

- **Option2**: Improve the design of the reflector and moderators: both in the geometry configuration and in the material selections. This strategy could be better focused on the “useful” neutrons rather than on the total neutron rate.
Option 1

INCREASING THE PRIMARY PROTON ENERGY
Doubling the proton energy, but keeping unchanged the total power deposited in the target, would lead to an increase of the integrated neutron rate of about 20%.

Keeping the proton energy unmodified (i.e. 800 MeV) but doubling the power deposition in the target would increase of about 60% the neutron yield (from 5 to about 13 n/pr).

but more severe engineering constraints have to be considered for the design (i.e. more severe heat transfer, neutrons shielding constraints)
Option 2

A SYNERGIC DESIGN OF TRAM AND NEUTRON BEAM LINES
FLAGGING NEUTRONS THROUGH MODERATORS

Asym. pois. water moderator
flag1= 131

Sym. pois. water moderator
flag1= 130

Liquid CH₄
flag2 151

Liquid Hydrogen
flag2 150

flag2 150
Liquid Hydrogen

flag2 151
Liquid CH₄
ESCAPING “FLAGGED” NEUTRONS

flag1=150,151 flag1=0, flag3=0
Ideal on lower beam ports

flag1=130,131, flag2=0, flag3=0
Ideal on upper beam ports

flag2=150,151 flag1=0, flag3=0
Ideal on lower beam ports

flag3=461 (Regions)
Be reflector or Boral liners
TRACKING THE TRAM ESCAPING NEUTRONS:
ANCESTORS, ORIGIN REGIONS AND "VISITED" MODERATORS
NEUTRONS ESCAPING THE TRAM: ORIGIN'S MATERIAL AND PARENT PARTICLES

TRAM (percentages wrt escaping neutrons):

- 67.8% are born in W
- 14.6% are born in Ta
- 13% are born in Be (by second. neutrons)
- 2.5% are born in SS
- 2.1% other

Passed through Water moderators: 7.9%
TUNGSTEN PLATE CONTRIBUTION TO WATER MODERATOR “FLAGGED” NEUTRONS

- W plate contribution to the neutrons escaping the TRAM: 68% of total escaping
- Of the TRAM escaping W-plate-generated neutrons only about 6% have passed through the water moderators
**NEUTRON ESCAPING BARE TARGET: ANGULAR DISTRIBUTION**

- **Very few** high energy neutrons (E> 100 MeV) escaping **backward**, because mainly emitted forward.
- The **side cylindrical surface** contributes to the overall neutron leakage by almost **83%** of the total.
- The **side leakage** is made mainly of neutrons coming from the evaporation stage (Maxwellian distribution around 0.7 MeV) of the heavy fragments in the spallation process, while only few of them (about 7% of the side leakage) have energy higher than 20 MeV and are produced by direct spallation process.
- The **backward current** is about **11.5%** of the total leakage and **does not exhibit the peak** around 100 MeV, while the **neutron leakage forward** is less than **6%** of the total.
- These results are obtained simulating only the target without reflector and moderators.
SOME PRELIMINARY ESTIMATIONS FOR BEAM LINES

POLARIS AND MAPS
The ISIS accelerator has been upgraded to achieve the ever increasing international demand for neutrons from the synchrotron to TS-2. In addition, the paper will summarise the substantial upgrades that have had to be made elsewhere on the ISIS accelerator system to meet the needs of significant increases in fluxes of moderated neutrons. In the initial phase a suite of seven instruments has been built, providing new opportunities in surface science, magnetic diffraction, small-angle neutron scattering and neutron scattering has been built, providing new moderators to be placed very close to the primary target, leading to significant gains in fluxes of moderated neutrons. In the initial phase a suite of seven instruments has been built, providing new moderators to be placed very close to the primary target, leading to significant gains in fluxes of moderated neutrons.

**Abstract**

The ISIS neutron producing target (TS-1) is driven by a 50 Hz, 800 MeV, 200 µA proton beam from a proton beam to TS-2 at the same time as maintaining the increased beam intensity necessary to provide a 10 pps in instruments are scheduled to begin in October 2008. First experiments on the new harmonic RF system for the ISIS synchrotron which will address possible future upgrades.

**The New ISIS Second Target Station (TS-2)**


**Background**

For neutron scattering has been built, providing new opportunities in surface science, magnetic diffraction, small-angle neutron scattering and neutron scattering has been built, providing new moderators to be placed very close to the primary target, leading to significant gains in fluxes of moderated neutrons. In the initial phase a suite of seven instruments has been built, providing new moderators to be placed very close to the primary target, leading to significant gains in fluxes of moderated neutrons.

**Materials and Methods**

The RFQ Accelerator

The RFQ Accelerator was built at Frankfurt University as part of the ISIS Upgrade Project. The 4-rod 202.5 MHz RFQ is installed on ISIS in 2004. The 4-rod 202.5 MHz RFQ is driven by ~200 kW (peak) of RF from a Burle 4616 fundamental RF cavities [4].

**Results**

The schematic layout of the central TRAM system, including TS-1 and TS-2, and also the transmission efficiency (compared with about 60% for the ISIS DTL). It is this increase in acceptance of the ISIS DTL. It is this increase in acceptance of the ISIS DTL. It is this increase in acceptance of the ISIS DTL.

**Discussion**

The ever increasing international demand for neutrons driven by a 50 Hz, 800 MeV, 200 µA proton beam from a proton beam to TS-2 at the same time as maintaining the increased beam intensity necessary to provide a 10 pps in instruments are scheduled to begin in October 2008. First experiments on the new harmonic RF system for the ISIS synchrotron which will address possible future upgrades.

**Conclusion**

The new ISIS Second Target Station (TS-2) represents a major enhancement of the ISIS spallation neutron source, and correspondingly major enhancements have had to be made to the accelerator system. As well as providing an outline of the new target station itself, this paper will describe the new dual transport line which diverts one out of every five pulses from the synchrotron to TS-2.
POLARIS AND MAPS

POLARIS instrument at ISIS is a high intensity, medium resolution powder diffractometer. It is optimised for the rapid characterisation of structures, the study of small amounts of materials (as little as ~1mm³), the collection of data sets in rapid time (with data collection times down to ~5 minutes) and the study of materials under non-ambient conditions.

MAPS has been in operation since 2000. It was the first chopper spectrometer to employ a large array of position sensitive detectors and the first to be designed solely for the purpose of measuring excitations in single crystals. A significant proportion of the beam time is devoted to single crystal excitation experiments involving the use of thermal neutrons, measuring excitations with energies as low as a few meV.
NEUTRONS INTO POLARIS
ENERGY SPECTRUM OF NEUTRONS IN POLARIS INLET

- **INLET**: (Part/pr) $2.06E-3 \pm 1.267\%$
- 0.04\% is the fraction of total TRAM escaping neutrons arriving on Polaris:
- Among those neutrons: 36.6\% are below 1 keV; 63.4\% above 1 keV;
- 16.25\% of all the impinging neutrons on Polaris have been flagged 131 (ASYM. POIS. WATER MODERATOR)

These results have been obtained by using blackhole material around the beam line. This provides the best optimistic scenario of useful “uncontaminated” neutrons coming from TRAM and channeling into the Polaris beam line.
POLARIS INLET: DETAILED TARGET PLATE CONTRIBUTION

W plates contribution to the neutrons arriving onto Polaris Port

- Normalised values with respect to the total arriving into Polaris port
- The contribution from secondary neutrons become predominant in the last 3 plates
POLARIS NEUTRON TRANSMISSION

- **16.25%** of all the impinging neutrons on Polaris have been flagged **131 (asym. pois. water moderator)**
- **1.4%** of all impinging neutron on Polaris have been flagged **151 (Liquid Hydrogen moderator)**
- **340 cm** far away from the inlet port the neutrons channeled are mostly flagged **131**

82% of the channeled neutrons are flagged **131**

Normalization is respect to total neutrons impinging into Polaris.
Neutron channeled in Polaris at 340 cm from the inlet have been generated mainly by direct spallation in the central target plates (any contribution form plates n.8 to 10).

72% of the channeled neutrons in Polaris have been produced in W. A not negligible contribution comes from Be born neutrons.
But actually all the 131 flagged neutrons that are channeled in POLARIS have passed by the Beryllium region after “visiting” the asymmetric poisoned water moderator regions and before leaving the TRAM

Ideal for instruments supposed to be served by water moderators

flag1=131, flag2 =0
FLAG3= 461

“VISA” of channeled neutrons in POLARIS as estimated by FLUKA

flag1=130,131 flag2=0, flag3=0
Ideal on upper beam ports
Most of the 131 flagged neutrons (asym. poi.water moderator) come from region n. 601 (boral moderator decoupler) and n.616 (Boral liner): that is, after having been in the asymmetric water moderator, neutrons pass across those regions before leaving the TRAM in their flight toward POLARIS inlet port.
ENERGY SPECTRUM OF NEUTRONS IN MAPS INLET

- **INLET**: (Part/pr) $1.789E-3 \pm 0.6\%$
- **0.035\%** is the fraction of total TRAM escaping neutrons that arrives on Maps INLET.
- **INLET**: **17.13\%** of all the impinging neutrons on Polaris have been flagged **131 (asym. pois. water moderator)**
- **77.87\%** of transmitted neutrons (at 340 cm) are flagged.... BUT... **only 131 (asym. pois. water moderator)**
- Note: only very few “130” (sym. pois. water moderators) neutrons are transmitted into Maps.

These results have been obtained by using blackhole material all around the beam line hole. This provides the best optimistic scenario of useful “uncontaminated” neutrons coming from TRAM and channeling into the Maps beam line.
CONCLUSION AND FUTURE PLAN

- Exploiting high performance computing resources and advanced Monte Carlo code skills, it is possible to track the escaping neutrons by transporting relevant information of their history (ancestors origin region, last TRAM region crossed before leaving, moderator "visited"...)
- Some preliminary estimations have been provided for the total TRAM leakage and for couple of instrument beam lines (Polaris and Maps)
- A more systematic and complete analysis is ongoing for all the instruments of ISIS-TS1 and a suitable complete postprocessing tool is under development (based on Matlab)
- The main goal is to provide useful hints to be studied and analysed for a more efficient TRAM design and/or for providing a valuable support for instrument scientist to assess quantitatively the effects of possible upgrading actions in the TRAM
Thank you for your attention!

https://www.isis.stfc.ac.uk/

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