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Neutronics modelling for the ISIS TS-1 upgrade

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Abstract. Following the successful validation of the current ISIS target station 1 (TS-1) neutronics model, the objective of this work is to re-assess the target, reflector and moderators (TRAM) assembly of the ISIS TS-1 to determine the possible improvements available by replacing these components. The goal is to deliver an upgrade model which improves the scientific output from all neutron beamlines, provides the largest collective gain, keep the instruments pulse time characteristics within the limits provided by instrument scientists, and can be built with minimum risk. A number of the MCNPX models of the TS-1 future TRAM assembly have been prepared by ISIS neutronics team. The new models have been optimized as part of the CombLayer package allowing extensive parametric and component selection without compromising the detailed engineering requirement. The upgrade models have been benchmarked against a baseline TS-1 model taking into account flux and time distribution of all existing TS-1 instruments. The best model shows that significant benefits can be achieved without modification to existing instruments, making the upgrade a low risk project.

1. Introduction

The Target Station 1 (TS-1) at ISIS operates very successfully for almost three decades. However, with the knowledge and computational tools now available it is widely believed that the neutronic output, efficiency and reliability of the TS-1 can be significantly improved. This was the reason to start a feasibility study of the potential TS-1 upgrade. Within the scope of the project, the proton beam delivered to the target is planed to be as it currently is: 800 MeV protons, beam current[1] of 180 μA and approximately double Gaussian profile with $\sigma_x = \sigma_y =$ 1.8 cm. The repetition rate is 50 Hz but every fifth pulse is delivered to the Target Station 2. Because re-configuration of the instruments (and the corresponding beamlines) is not a likely option, the project has been focused on re-assessing the TS-1 target, reflector and moderator (TRAM) assembly. In reviewing the risks, the TS-1 upgrade project has been defined as a reasonably conservative, driven by the fact that TS-1 is already operating, and compromising existing performance of the instrument suite in either flux or availability needs to be negligible [1].

The procedure for neutronics part of the project was, as a first, to create a robust, detailed neutronics model of the current TS1 (*baseline*) with idea to validate the neutronics reliability after review of simulation results and comparison with experimental results. The next step was to establish and then maintain a number of simulation models of the TS-1 zone which includes future TRAM assembly and current void vessel, beamlines, bulk shielding, etc. The

[1] There is a possibility to increase the beam current to 200 μA.

CombLayer tool [2] has been used for construction and optimisation of all these models (ultra-rapid prototype models, detailed models that establish beamline performance and selected high specification models for specialized types of calculations). The new models have been benchmarked against a baseline TS-1 model taking into account flux and time distribution of all existing TS-1 instruments. The main results of this neutronics study and TS-1 upgrade optimisation are presented in the following sections.

2. Current ISIS TS-1 model

The cross-sections of the TS-1 TRAM assembly are shown in Figure 1. The target consists of tantalum cladded tungsten plates. There is 12 tungsten plates with different thicknesses: 1.1, 1.1, 1.2, 1.35, 1.5, 1.8, 2.1, 2.6, 3.4, 4.0, 4.6 and 4.6 cm. The height of the tungsten plates is 4.0 cm and the width is 5.25 cm. The thickness of tantalum cladding is 0.2 cm. Target pressure vessel is made of stainless steel and the target is cooled with heavy water. The water channels width is 0.2 cm.

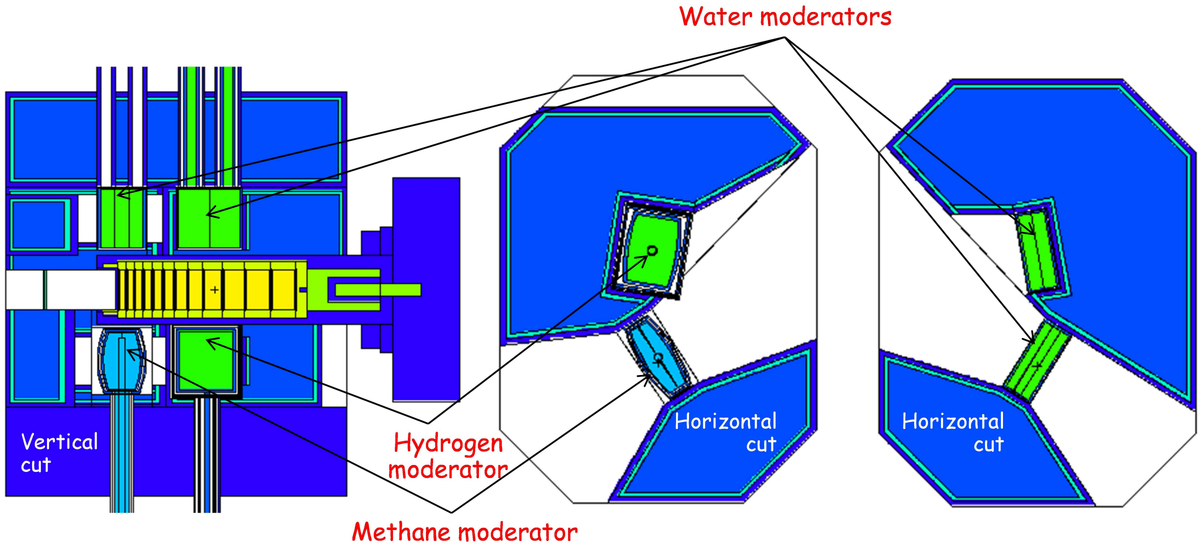

Figure 1. MCNPX model of current ISIS Target Station 1 TRAM assembly.

The reflector is made of beryllium rods cooled with heavy water (packing fraction = 90:10 by volume). The reflector size is: 83 cm (height) x 52 cm (width) x 70 cm (thickness).

Currently there are four moderators at the TS-1. Two water moderators operating at room temperature are located above the target (see Figure 1). The first water moderator has two poison (gadolinium) layers, the second one has a single poison layer. These two moderators are identical in size: 12 cm (height) x 12.5 cm (width) x 4.5 cm (thickness). The poison layer thickness is 0.005 cm. Below the target there are liquid hydrogen moderator and the liquid methane moderator (see Figure 1). Hydrogen moderator operates at 20 K with assumed composition: 80% para-hydrogen : 20% ortho-hydrogen. The hydrogen moderator size is: 12 cm (height) x 11 cm (width) x 8 cm (thickness). Liquid methane moderator operates at 110 K, and it is centrally poisoned with a single, 0.005 cm thick, gadolinium layer. The methane moderator size is: 11.5 cm (height) x 12 cm (width) x 4.5 cm (thickness). The neutron flightlines are lined with, 0.65 cm thick, boral layers. The same material is used as the moderators decoupler.

These four moderators serve 17 beamlines at ISIS target station 1 (see Figures 2 and 3) and provide neutrons for the experiments in the fields of spectroscopy (MAPS, MARI, MERLIN), molecular spectroscopy (IRIS, OSIRIS, TOSCA, VESUVIO), large scale structures (CRISP, SURF, LOQ), diffraction (HRPD, SXD, POLARIS, GEM, PEARL), disordered materials (SANDALS), etc. These different instruments have different priorities that have to be fulfilled. For example POLARIS, TOSCA, GEM, HRPD and PEARL are sensitive to pulse width while MAPS, VESUVIO, SXD, MERLIN, SURF, CRISP, LOQ and IRIS can accept "relaxed" pulse width if this is a condition to have bigger flux gain. All these requests, of course, constrain the neutronics optimisation.

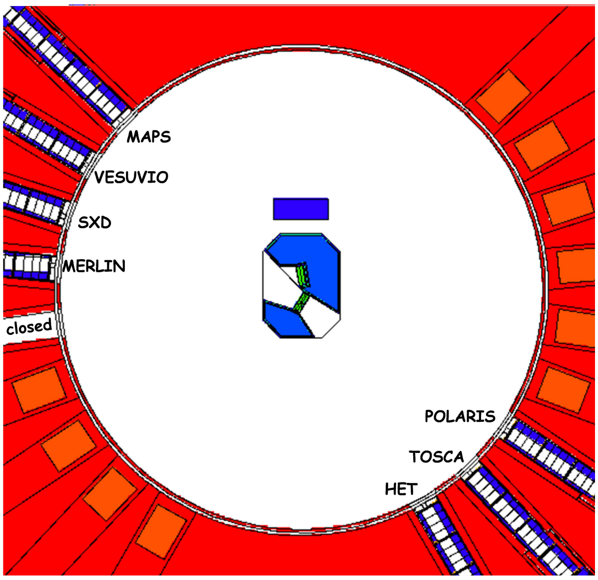

Figure 2. MCNPX model of current ISIS Target Station 1: The beamlines for water moderators.

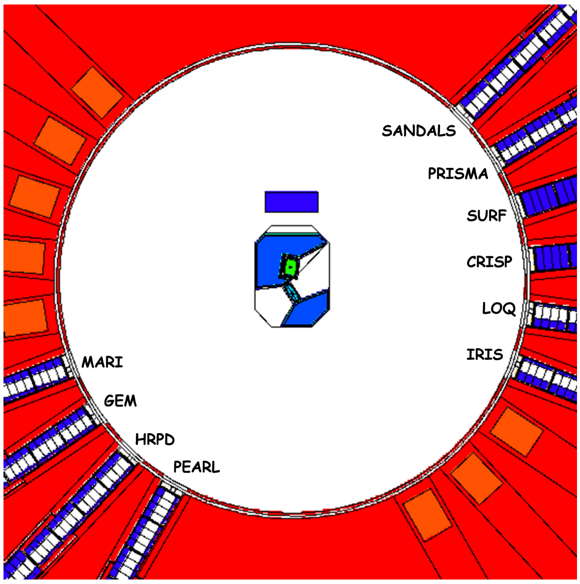

Figure 3. MCNPX model of current ISIS Target Station 1: The beamlines for cold moderators.

The CombLayer tool has been used to build MCNPX [3] model of the Target Station 1. Next step was to calculate neutron spectrum (for each beamline) using a point detector placed 10 m down each flight path, viewing the corresponding moderator through the modeled collimation within the bulk shield. It can be seen in Figures 2 and 3 that the model of the beamlines shutter inserts is very detailed. This is necessary not only for comparison with experimental data but also to allow accurate comparison with the upgrade model because the beamlines will remain the same. The CEM03 physics model [4] and ENDF/B-VII cross-section library [5] have been used in these simulations. In addition to this, the McStas [6, 7] input files have been prepared to help instrument scientists to trace down neutrons to the sample/detector positions and to compare the obtained results with experimental data. Very nice agreement between TS1 Baseline model results and experiments has been found (see [8] for more details). The comparison with the experiments helped also to resolve some issues in the knowledge of the current TS-1 performance[2].

3. The TS-1 upgrade models

The neutronics part of the TS-1 upgrade project has been driven by the idea to get a gain through a combination of (relatively) small changes in the TS-1 TRAM rather than through a single dramatic change in concept which could increase the project risk level. A number of

[2] For example, the para-hydrogen/ortho-hydrogen ratio in the hydrogen moderator has been estimated by matching the shape of the experimental time-of-flight data from the OSIRIS instrument [8].

TS-1 upgrade models have been produced using the CombLayer tool and for each model the performance is compared with the baseline model (over full TS-1 instrument suite).

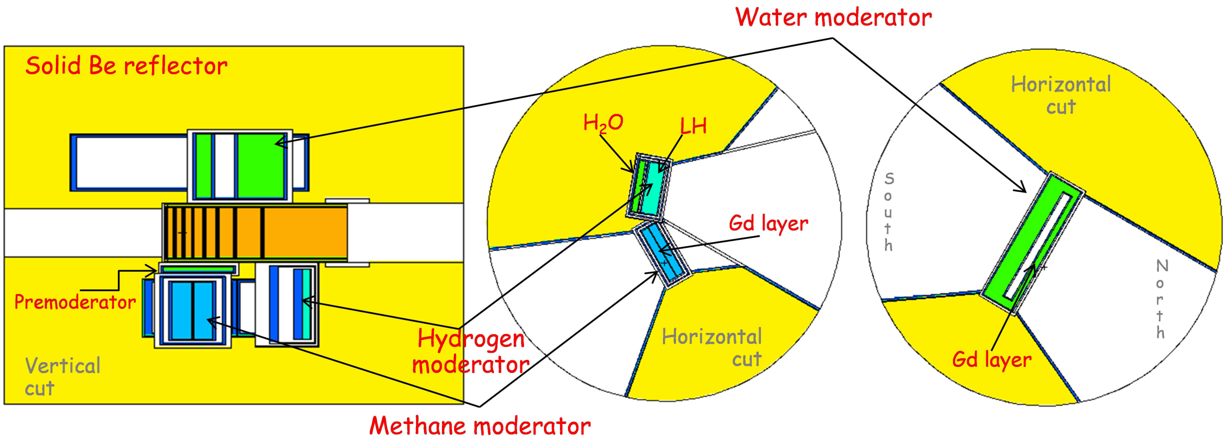

Figure 4. MCNPX model of the proposed TRAM assembly for ISIS Target Station 1.

The neutron flux ratios are calculated by taking the same tally point for each instrument and placing the different model (upgrade and baseline) in the void vessel and dividing the integrated flux. The pulse time shapes were also analysed and compared with the corresponding baseline results. The cross-sections of the final TS-1 upgrade model is shown in Figure 4 and the list of changes can be summarized as follows:

3.1. Target and reflector

The new target design is similar to current, operating TS-1 target. The main differences are that the target cross section is changed to be cylindrical (with core radius of 4.9 cm) and that target housing material is changed from stainless steel to tantalum (thickness of tantalum pressure vessel is 0.3 cm). The target is still based on tantalum-clad tungsten plates with 0.2 cm thick water (D_2O) channels between them. Tantalum cladding thickness remains 0.2 cm. The thicknesses and the number of plates have been optimised for three different beam currents: 180 (default), 240 and 300 μA. It is shown that number of plates increases with increasing beam current from 8 at 180 μA, to 10 at 240 μA and finally to 12 plates at 300 μA [9]. For the default beam current the thicknesses of eight tungsten plates are: 1, 1.1, 1.3, 1.6, 2.1, 2.8, 4.7 and 16.4 cm. The change of the reflector is based on replacing the stainless steel vessel filled with beryllium rods to a solid, edge-cooled beryllium structure. A new reflector has a cylindrical shape of 45 cm in radius and it is 70 cm high.

3.2. Cryogenic moderators

Hydrogen moderator is now a composite moderator, it has a liquid hydrogen layer backed with a water layer which serve as a pre-moderator. The liquid hydrogen part of this composite moderator operates at 20 K, with assumed para-ortho hydrogen composition of 80 : 20 to match a baseline model. Its size is 13.8 cm (height) x 14.2 cm (width) x 4 cm (thickness). The thickness of water (pre-)moderator is 1.5 cm and it operates at room temperature.

The gain factors for instruments looking at the hydrogen (composite) moderator are shown in Figure 5. The composite moderator makes gains due to the mixed LH+H_2O design. It is well known that looking into the pre-moderator of a hydrogen moderator increases the flux and this is exploited here. However, because the pulse width has to be matched, the amount of pre-moderator has been limited, so effectively it was a study of the optimal place to put the pre-moderator.

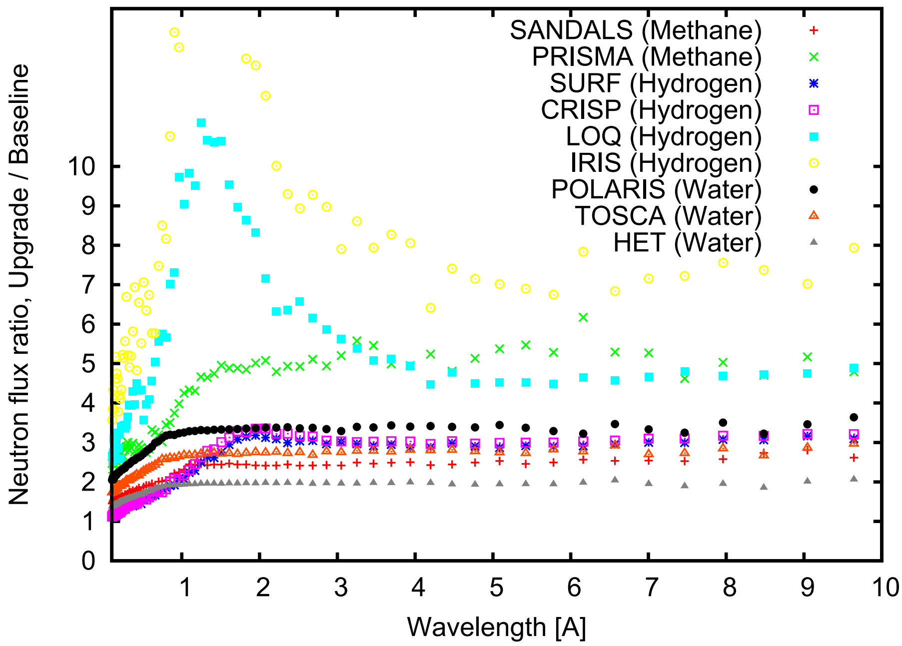

Figure 5. Gain factors for the north side beamlines/instruments.

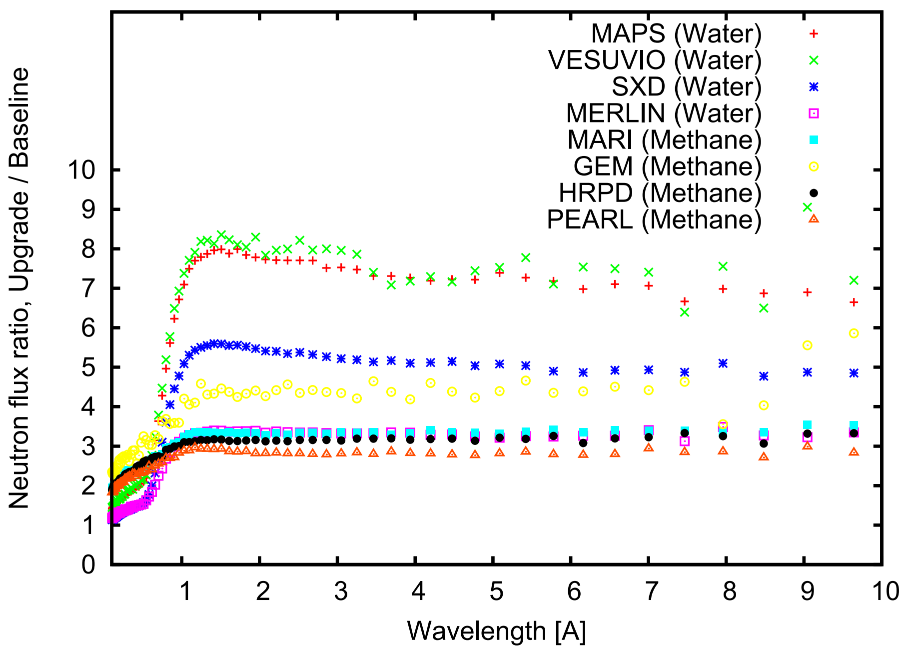

Figure 6. Gain factors for the south side beamlines/instruments.

The ratio of the pulse shape widths ('full width at half maximum' - FWHM's) for upgrade and baseline design of cryogenic moderators is shown in Figure 7 for different beamlines/instruments.

It can be seen that a significant portion of the gain in the case of a new hydrogen moderator is obtained by relaxing the pulse width by $\sim 25\%$ in the wavelength region of interest (around 6 Å). Additionally, non-negligible gains have been obtained due to the history, where originally, only two instruments were going to look at the hydrogen moderator. This is corrected here by putting the moderator in a better position for all those that view it.

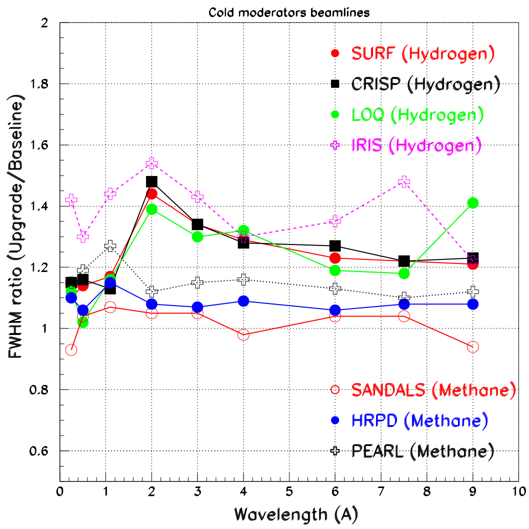

Figure 7. The ratio of the pulse shape widths (FWHM's) for upgrade and baseline design of cryogenic moderators.

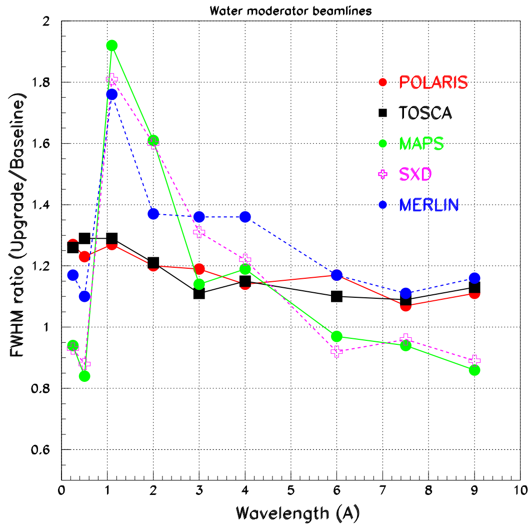

Figure 8. The ratio of the pulse shape widths (FWHM's) for upgrade and baseline design of water moderators.

Liquid methane moderator is practically identical in shape and size to the baseline methane moderator (11 cm (height) x 14 cm (width) x 4 cm (thickness)). It operates at 110 K and has a single poison (Gd) layer. However, the significant difference is that there is a 1 cm thick ambient water pre-moderator between target and liquid methane moderator. The gain factors for instruments looking at the methane moderator are shown in Figures 5 and 6. The methane moderator makes gains because of slightly better target position, the relaxation of the pulse widths for $\sim 10\%$ in the useful wavelength ranges (see Figure 7), and use of solid beryllium reflector and pre-moderator. Also, two cryogenic moderators have been moved closer to the target hot spot, allowing them to be (partially) pre-moderators to each other. In addition to these, boral liners and decouplers have been replaced with cadmium and the decouplers around the perimeter of all the moderators have been completely removed.

3.3. Water moderator

Two water moderators in current TS-1 configuration have been replaced with a single water moderator, operating at room temperature. The moderator height is 12.6 cm and width is 35.2 cm. The thickness of the water layer on south side is 4 cm and the moderator has 2 cm thick hole in the middle to partially control pulse width at south side. The instruments looking at this side of the water moderator (MAPS, SXD, MERLIN) are ready to significantly relax the pulse widths (illustrated in Figure 8) in exchange for bigger gains shown in Figure 6.

A single poison (Gd) layer has been added on the north side and the optimal thickness of the water layer on this side has been found to be 1.5 cm. The POLARIS and TOSCA instruments request that pulse widths should not be relaxed for more than $\sim 25\%$ (see Figure 8) resulted in the gain factors shown in Figure 5.

4. Conclusions

The aim of this study was to determine possible improvements of ISIS target station 1 by re-configuring the target, reflector and moderators assembly. Following the successful validation of the current TS-1 neutronics model, a number of the MCNPX models of the TS-1 future TRAM assembly has been prepared using the CombLayer tool. The neutronic output has been optimised across the existing TS-1 (and foreseeable future) instrumentation to produce the largest collective performance gain.

During the optimisation process, instrument scientists have been considered as the 'owners' of a performance metric for the neutronic output of their beamline and it is their metric which allowed ISIS neutronics team to perform optimisation of the upgrade models. For example, as one of the initial requests, most of the instrument scientists preferred to see no or limited pulse broadening within their respective useful wavelength ranges. Keeping all these constraints and requests in mind, significant gains are predicted through a combination of proposed changes (described in Section 3). Together, these changes lead to average flux gain of 3.4. It should be noted that some of the gain is a result of reduction of the amount of poisoning and decoupling while about an average factor of 2.2 (as seen by the epithermal gain) is purely due to re-configuration of the TS-1 TRAM.

The next step within the TS-1 upgrade project is to create and critically review a robust engineering analysis of the potential gains and risks involved in the upgrade scenario. It is expected that results of this process will change the gain factors. However, proposed neutronics model of the upgraded TS-1 TRAM contains sufficient engineering reality (cooling channels, clearance gaps, shutter inserts, etc.) to allow reasonably accurate prediction.

References

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