SNS Second Target Station Moderator Studies

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Abstract. Moderator performance studies were conducted to scope out conceptual target-moderator-reflector configurations for a second SNS target station (STS) for providing long-wavelength pulsed neutron beams with prime peak brightness. STS was assumed to receive 467 kW proton beam power at 1.3 GeV proton energy in short-pulse structure (<1 us pulse length) at 10 Hz repetition rate into a stationary compact solid tungsten target with a flat proton beam of 30 cm² footprint. Coupled cylindrical supercritical para-hydrogen moderators with ambient water pre-moderators with three neutron extraction ports were investigated for neutron scattering instruments needing peak intensity beams; box-shaped decoupled centrally poisoned para-hydrogen moderators were investigated for high-resolution instruments. We optimized the configurations of coupled and decoupled moderators with the square viewed areas ranging from the standard-size 10x10 cm² down to the smallest size of 2x2 cm² viewed areas to arrive at optimized cold neutron pulse peak brightness using MCNPX imbedded into global optimizer framework. With this body of information and a requirement to feed a suite of 19 STS candidate instruments we tailored a STS moderator suite to feed a suite of 19 candidate STS instruments consisting of a flat 3cm high coupled cylindrical para-hydrogen moderator, a box-type coupled para-hydrogen moderator with 5x5 cm² cross sectional area and 10 cm depth, and a decoupled moderator unit with a cold para-hydrogen side and an ambient water side. For the coupled cold moderators, gains in peak brightness of a factor of 11-13 were demonstrated comparing to the first target station coupled moderators operated at 2 MW and 50 Hz; for the decoupled moderators the STS gains in peak brightness were a factor of 3-4.

1. Introduction
Oak Ridge National Laboratory is pursuing conceptual design work on a second target station (STS) with the goal to supplement its suite of instruments with complementary capabilities as outlined in the STS Technical Design Report [1]. The second target station is seen as an opportunity to address next-generation science challenges. Profiting from the technological progress in neutron optics developments and to adapt to the requirements of smaller samples, longer length-scales of structures and investigation of dynamic systems, our goal is to design instrumentation that exceeds the capabilities of present day instrumentation by orders of magnitude and opens the door to new science. Improvements of the instrumentation are to be harvested from the optimizing the source (target/moderator/reflector) through optics to detectors. The gains achievable by the source are discussed in this paper.

Earlier efforts of STS investigated the long-pulse option utilizing every third pulse of the SNS accelerator system circumventing the accumulator ring arriving at about 1MW beam power at 20 Hz repetition rate and 1 ms pulse length [2]. Considering the inferiority of such a source in comparison with ESS operated at 5 MW, and learning about the successes of the highly optimized ISIS TS2 [3] operated in the short-pulse mode, encouraged us to explore in more depth the STS short-pulse option.
2. Target Station Concepts
The source performance derives from the right material choices of target, moderators and reflector [4] and their tight coupling and the beam parameters. Building on the existing SNS accelerator that already has shown its ability to deliver a 1.4 MW proton beam at 1 GeV proton energy, 60 Hz repetition rate and 0.7 μs pulse length, we foresee a build-out of the accelerator system to 2.8 MW and 1.3 GeV beam energy. Every sixth pulse is in a pulse-stealing mode routed to STS, which hence would operate at 467 kW and 10 Hz repetition rate. The lower power will allow us to inject the beam into the target at a beam footprint area of 30 cm². The remainder of the pulses would drive the first target station (FTS) at 50 Hz repetition rate in a 60 Hz time structure. We also assume here that FTS is limited to 2MW power.

Building on the expertise of spallation source technologies tested and proven in facilities at IPNS, ISIS, Lujan Center, SNS and JPARC, we choose a heavy-water cooled stacked plate tungsten target as spallation target because of the superior material density and the resulting large neutron yield in a very compact neutron production zone. For coupled cold moderators, para-hydrogen pre-moderated with light water is the prime choice for highest-intensity cold beam generation at a mega-watt facility [5]. Also for a decoupled moderator, para-hydrogen is a good choice. Liquid carbon-hydrates suffer from polymerization and subsequent clogging up of supply piping and do not offer better performance. Solid carbon hydrates (mesithylene, methane) are in use at IBR2, loose their advantage of the higher hydrogen density when used in the pelletized from. In the solid monolithic form as in use at ISIS TS2, the moderator would have to be regenerated at least 10 times more frequently to avoid the violent release of accumulated energy caused by the radiation-induced breaking of molecular bonds.

For a reflector, the unanimous pick is beryllium, a good moderator of its own right and a material with good thermal and mechanical properties.

3. Moderator Performance Studies
The increasing complexity of materials being studied at photon and neutron sources are being synthesized in elaborate procedures, which result in a reduction of available sample masses and sizes for scattering experiments. Striving for unchanged instrument resolution, the neutrons from a given fixed source size cannot be focused down to a smaller sample without degradation of the experiment and are of no use in the experiment. As has been pointed out by Zhao [6] and Carpenter [7], the source size and instrument optics has to be matched to the sample size. On the other side, the neutron brightness varies greatly across the viewed moderator face dependent on the wavelength range, moderator choice but also dependent on target/moderator geometry as demonstrated by Lu [8] for the SNS FTS moderators. These findings were actually exploited by the instruments EQSANS [9] and NSE [10] and with limited moderator view to align their optics off-moderator-center to utilize higher moderator brightness and hence gain fluxes at sample of factors of 1.5. If instruments are not utilizing the full view of the moderator, the moderator size can be reduced with gains of moderator brightness (to be shown), but also result in a lower hydrogen inventory, in a smaller integral cryogenic heat load and consequently reduced construction and operations cost.

While we were exploring these options for a short-pulse system for coupled and decoupled moderators, ESS did likewise for the long-pulse target station and indeed published interesting findings of gains that match in broad terms our results [11].

Details of our principal work, optimization studies of moderators on compact tungsten targets, surrounded by beryllium reflector, involve MCNPX [12] as the tool to assess moderator performance and are described in an extensive report [13] and in a publication in preparation [14].

Without going into detail here, the findings are summarized as follows.

For cylindrical coupled para-hydrogen moderators with light water pre-moderator and neutron extraction at three ports of a given square-sized neutron extraction ports, the moderator dimensions, pre-moderator dimensions, proton beam and consequently target height at a given proton beam footprint of 30 cm² (flat beam distribution), and moderator position with regard to target nose were optimized with respect to a figure-of-merit emphasizing peak brightness below 5 meV of neutron
energy. Moderators with viewed areas ranging from 10 x 10 cm² to 2 x 2 cm² were investigated. For the resulting optimized configurations extended moderator performance assessments were conducted, the results of which are shown in figure 1 for peak brightness and figure 2 for brightness integrated over one pulse. The analyses for FTS and STS assumed equal energy pulses, however, the proton energies assumed 1 GeV for FTS and 1.3 GeV for STS.

The STS moderator with viewed area 10 x 10 cm² closest matches the FTS moderators, which all have viewed areas of 10 cm width and 12 cm height. In the cold neutron range below 10 meV the pulse-integrated and peak pulse gains of the STS moderator are 7 and 5. A factor of four of the STS gains for the coupled moderator can be attributed to moving the moderator at the prime neutron production zone of the target and by having a moderator depth optimized to para-hydrogen. In contrast, the FTS coupled moderators are located downstream of the decoupled moderators at a distance from the prime neutron production and were dimensioned to 5 cm depth to make them fairly insensitive to ortho-para fluctuations of the uncatalized hydrogen loop. With these choices, the FTS coupled moderators suffered greatly in performance as comparisons to the JPARC coupled moderator as indicated in Ref. [15]. The gains above four are to be attributed to the target choice, compact proton-beam footprint and better target/moderator coupling. Additional gains of a factor of 2.5 and 3 in pulse-integrated and peak brightness, respectively, are to be had over the STS configuration with 10 x 10 cm² viewed area. It is worth mentioning that with the selection of the peak-brightness FOM, the moderator radius reduced from 7.6 cm for the 10 x 10 cm² viewed area to 3.7 cm for the 2 x 2 cm² while the pre-moderator thickness increased from 1.5 cm to 2.8 cm. For a selection of a FOM favoring the pulse-integrated brightness the optimal moderator dimensions would certainly have resulted in larger radii and somewhat higher pulse-integral brightness values closer to what we found in the long-pulse studies [2].

Figure 1. Peak brightness gains over the FTS coupled moderator based on equal power pulses.
In a similar way, decoupled para-hydrogen moderator studies were conducted. The studied decoupled moderators were box-type moderator volumes, viewed from two opposite sides, centrally poisoned by gadolinium and decoupled from the beryllium reflector by cadmium layers around the not-viewed aluminum vessel walls and the square-sized neutron extraction ports. The optimization tuned the moderator dimensions, proton beam height at fixed proton beam area of 30 cm$^2$, and the moderator position with regard to the target nose. As the FOM, we used the neutron intensity below 10 meV energy within a pulse time window of energy-dependent width equivalent to the emission time FWHM value of the pulse of the FTS decoupled hydrogen moderator [8] and penalized by the neutron intensity outside of the time-window. Better-converged calculations were performed for the optimized configurations for each setting of viewed area. The moderator depths of 4.4 cm thickness obtained from the optimizations for all viewed area settings produced FWHM pulse widths that were somewhat narrower than that of the FTS moderator. For this reason the moderator thickness was increased to 5 cm for the production calculations, which arrived at better FWHM matches. The gains of peak brightness over the FTS decoupled hydrogen moderator [8] are shown in figure 3. Gains of a factor of 2.6 are obtained for cold neutrons for the STS moderator with 10x10 cm$^2$ viewed area. It seems that the overall smaller decoupled moderators benefit more from the small-footprint target and proton beam. The gains grow to a factor of 5 for the small STS version with 2x2 cm$^2$ viewed area, hence by almost a factor of 2 over the STS 10x10 cm$^2$ configuration.

Figure 2. Pulse-integrated brightness gains over the FTS coupled moderator based on equal-energy pulses.
4. Matching STS Instrument Needs to Moderators

These model simulations described in section 3 indicate that significant gains of neutron performance are to be had at STS over FTS. In parallel to these studies, an STS candidate instrument suite of 19 instruments was developed. The instrument developers requested the preferred type of moderator (coupled/decoupled), neutron spectrum (cold/thermal) and the viewed area size as summarized in Table 1. As only three to four moderators can be realized at a target station, choices of moderators and moderator characteristics have to be made. From Table 1 we conclude that the moderator with highest request is a coupled cold moderator with viewed area of 3x3 cm$^2$. Configuring the cylindrical para-hydrogen moderator with two viewed ports of 3x3 cm$^2$ and one port with 3x6 cm$^2$ (height x width), we still can maintain the flat moderator design and serve 11 instruments. In addition a larger–area coupled cold moderator is requested and essential to two instruments, which requires a second cold coupled moderator. Decoupled moderators of various sizes and with thermal and cold characteristics that are best met by a back-to-back para-hydrogen/ambient water decoupled moderator of viewed areas of 7x7 cm$^2$.

Table 1. Moderator characteristics as requested by the proposed STS instrument suite.

<table>
<thead>
<tr>
<th>Moderator type</th>
<th>View port size (cm)</th>
<th>Requested</th>
<th>Assigned</th>
</tr>
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<tbody>
<tr>
<td>Cold coupled</td>
<td>10x10</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>Cold coupled</td>
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<td>3</td>
</tr>
<tr>
<td>Cold coupled</td>
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<td>7</td>
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<tr>
<td>Cold coupled</td>
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<td>0</td>
<td>2</td>
</tr>
<tr>
<td>Cold decoupled</td>
<td>7x7</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Cold decoupled</td>
<td>5x5</td>
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<tr>
<td>Thermal-cold decoupled</td>
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<td>3</td>
</tr>
<tr>
<td>Thermal-cold decoupled</td>
<td>3x3</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>
5. First Try STS Moderator Suite
A first effort was undertaken to cast the thoughts of the previous chapter into a moderator suite for a technical design report (TDR). In this design depicted in figure 4 the target structure was refined by a 19 tungsten plate structure, which resulted from thermal heat removal considerations. The cylindrical para-hydrogen moderator was placed at the bottom of the target (B), a box-type coupled para-hydrogen moderator at the top upstream position (TU) with 5x5 cm² viewed area, and a decoupled moderator unit consisting of ambient water and decoupled para-hydrogen moderators at the top downstream position (TD) each with 7x7 cm² viewed area. To arrive at optimal positions and dimensions, the bottom moderator was optimized first, followed by the coupled cold moderator in the top-upstream position, both using the peak cold brightness FOM mentioned above. Before putting our attention to the decoupled moderator unit, the sensitivity of the performance of the TU moderator with regard to displacement in upstream direction was assessed with the finding that a 3 cm shift cost only 5% of performance reduction. After applying the TU moderator shift, the decoupled TD moderator unit was optimized using the decoupled moderator FOM tailored to the FTS decoupled cold hydrogen and ambient water moderators, respectively. Naturally the optimizer moved the moderator as close as possible to the prime neutron production zone without interfering with the TU moderator.

![Figure 4. Arrangement of three moderators in wing configuration around the STS tungsten target.](image)

Again a final analysis was undertaken to arrive at fully converged moderator performance data. Results of peak brightness spectra are shown in figures 5 and 6 for the coupled and decoupled moderators, respectively. We were pleased to see that the TDR moderator performance held up to the promises of the single-moderator studies. The cylindrical para-hydrogen moderator saw only a single digit percentage loss mainly by adding the detailing of the target structures including cooling channels. The TU cold coupled moderator with 5x5 cm² viewed area increased its peak brightness by 10% over the single moderator studies despite the 5% loss from shifting it upstream, mostly because its shape was converted from a cylindrical to a box-type moderator with tighter coupling to the pre-moderator. The decoupled para-hydrogen moderator suffered only a 25% loss over the single-moderator results.
6. Conclusions

Despite adopting conservative, but proven choices for the material and design of the target/moderator/reflector assembly, an attractive target/moderator/reflector configuration is found. Optimization of moderator and premoderator dimensions, and moderator positions with regard to the target result in a configuration with a small proton beam footprint and tightly coupled target moderator with promising STS moderator performance. Brightness increases of a factor of 2-3 by downsizing the moderator viewed areas from 10x10 cm² to 2x2 cm² were demonstrated both for coupled and decoupled moderators. Gain factors on peak brightness of a factor of 13 were shown for STS at 467 kW beam power at 10 Hz compared to FTS operated at 2 MW and 50 Hz for a 3 cm high para-hydrogen cylindrical moderator. The gain factors for the STS decoupled moderators are 3 and 4 for the cold and thermal moderators, respectively. In this round of analyses, the optimizations were driven by crude empirical quantities based on peak brightness metrics. Ultimately, we are striving to refine the optimization strategies to involve instrument specific metrics to arrive at moderators that perfectly tailored to the instruments’ needs.

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Figure 5. STS-TDR peak brightness of the coupled cold moderators compared to the FTS cold moderators.
Figure 6. STS-TDR peak brightness of the decoupled cold and thermal moderators compared to the FTS moderators and compared to an optimized single STS para-hydrogen moderator.