Reproducing TDR and "Pancake" ESS brilliances using McStas

Peter Willendrup and Ken Andersen

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This document is meant to give further clarity on the available ESS source parameterisations for use with McStas. We shall only consider the TDR and pancake type brilliances, as these are ESS baseline quantities or considered important milestones. The "optimised thermal" moderator configuration is currently not implemented in McStas.

A new component called ESS_moderator.comp was distributed with McStas 2.1 and also exists for use with 2.0 and 1.12c through the archive

http://mcstas.org/download/share/ESS_moderator_July_2014.tgz

The component comes with a library of ESS source brilliances, each labeled:

- **2001**, legacy "Mezei moderators" from the original F. Mezei documents, rescaled to ESS TDR frequency, pulse-length and power.
- **TDR**, Mezei moderators, with a wavelength-dependent correction term to the cold flux, derived from 2012 MCNPX calculations by ESS neutronics group. Corrections calculated by K Lieutenant (Vitess) NOTE: uses the 2001 brilliance for the thermal moderator!
- **2013**, post-TDR update with non-Maxwellian cold spectrum, Troels Schoenfeldt, BEFORE the ESS pancake geometry was introduced.
- **2014** updated brilliance using formulation by Troels Schoenfeldt, including support for the "pancake", i.e. flat geometry and variation of the brilliance over the moderator surface.

Selecting one of these parameterisations defines **both** a cold and a thermal brightness, emitted from a dual-moderator surface with a cylindrical cold moderator and thermal wing slabs. The fraction of statistics emitted from each of these can be selected through the cold_frac parameter.

Optimised Thermal (OT) moderator or "butterfly" moderators:

These moderators are unfortunately not yet implemented in McStas. We advise to use the "2014" brilliance which is comparable but 10-50% lower in flux.

Pancake moderator:

A 3cm high "pancake" moderator is selected by choosing the parameter set

```
COMPONENT Source = ESS_moderator(dist=2,
            focus_xw=guidewidth, focus_yh=guideheight,
            Lmin=lambdamin, Lmax=lambdamax, cold_frac=0.5,
            sourcedef="2014", yheight_c=0.03, yheight_t=0.03)
AT (0, 0, 0) RELATIVE Origin
```

The following parameters can be adjusted from their defaults:

- 0 < cold_frac < 1 defines the fraction of statistics emitted from the cold source
- 0 < isleft < 1 defines the fraction of the thermal statistics which is emitted from the "left" (i.e. upstream w.r.t. the proton beam) thermal wing
- yheight_c and yheight_t are used to define the height of the pancake-moderator. The brilliance varies with this height.

When using the "2014" parameter set, the following parameter definitions are implicit:

- xwidth_c=0.23, xwidth_t=0.12 (the in-plane moderator geometry is fixed)
- extraction_opening=120 (the neutronics calculations were done at 120 degree extraction-area width)
- beamport_angle=60 (the angular emission variation is not yet implemented, but variation is expected to be relatively low ~10%)

Let us also have a quick look at the geometry - see Figure 1 on the right.

If your instrument is solely or mostly thermal, we advise the use of an Arm to control the orientation of the neutron optics with respect to the moderator ‘z’ axis which in the 2014 setting is the midpoint of the beam extraction.

The reasoning is that neutrons emitted from the thermal moderator ‘slabs’ are geometrically shifted with respect to the instrument axis. I.e. to effectively transport beams with a high proportion of thermal neutrons, you will need to add a rotation of your optical axis at the beamport position.

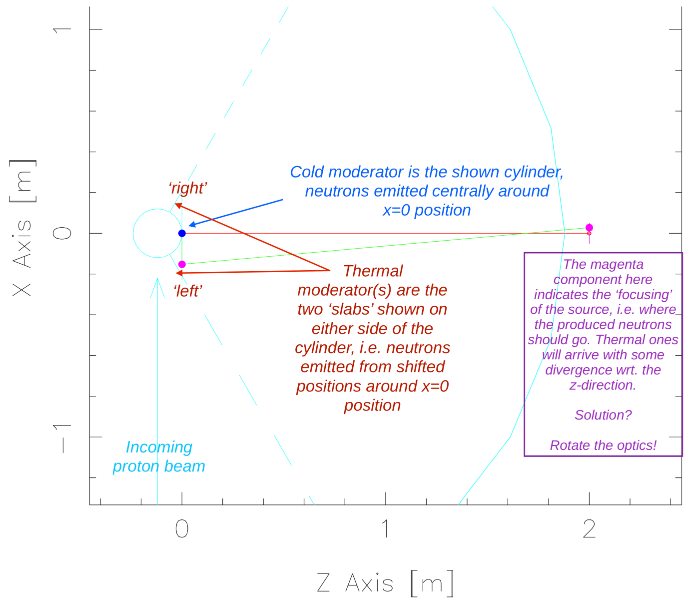


Figure 1: illustration of the geometry

In Figure 2 below, a moderator-setup with a mixture of thermal and cold neutrons has been selected, with thermal neutrons only emitted from the ‘left’ moderator slab. The shown monitor outputs give a) the spectrum and b) a wavelength-divergence diagram. The outputs on the left are measured *without* a rotation of the monitors, i.e. the thermal neutrons from the thermal slab give a peak at ~5 degrees. The outputs on the right shows that this can be rectified by a rotation of the monitors, here the output from the thermal slab is measured around the ~0 degree direction.

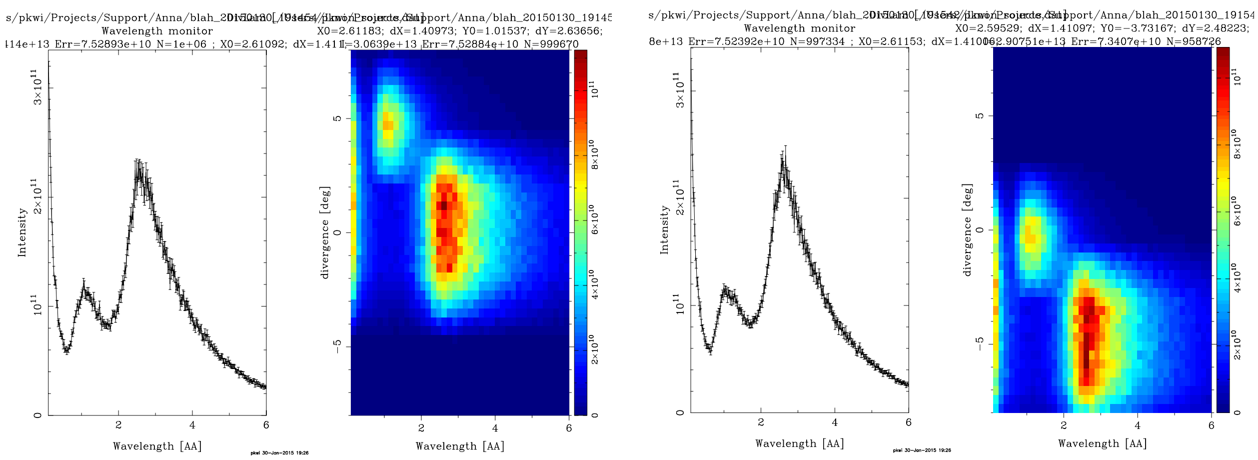


Figure 2: Illustration of the divergency-shift of neutrons from the ‘left’ thermal slab.

The left-most figures in Figures 3 and 4 below show fits and histograms of ESS neutronics data from the paper “Phenomenological Study of Expected Cold and Thermal Brightness Phase-Space at ESS” by Troels Schönfeldt et. al (in preparation). On the right part of the same figures, the corresponding McStas simulation output is shown (produced via the ESS_brilliance_2014 instrument file).

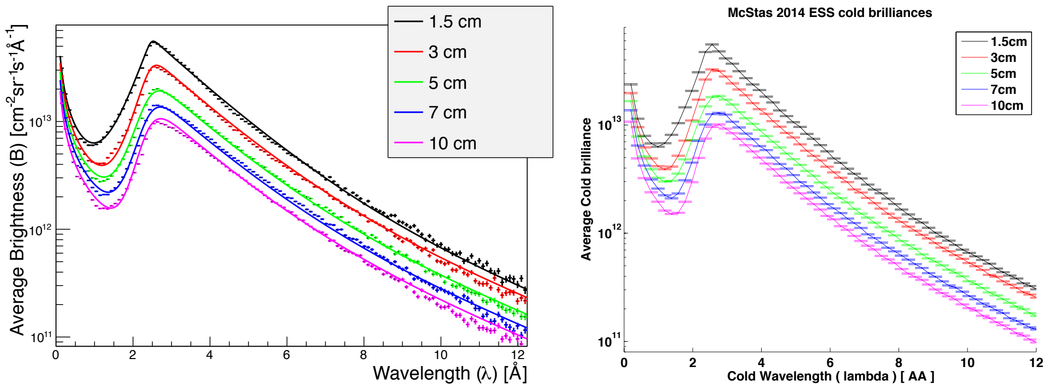


Figure 2: Cold brilliance from the “pancake” as function of moderator height. Left: MCNPX + fits Right: McStas 2.1 ESS_moderator.comp

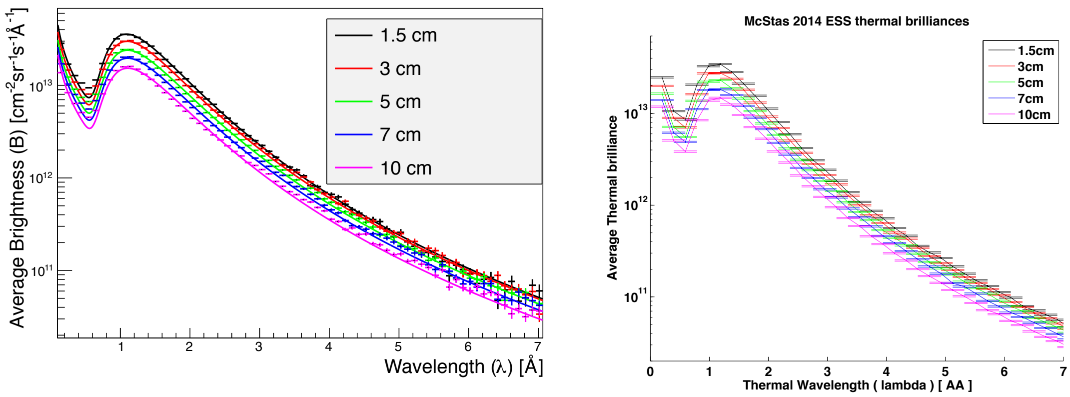


Figure 3: Thermal brilliance from the “pancake” as function of moderator height. Left: MCNPX + fits Right: McStas 2.1 ESS_moderator.comp

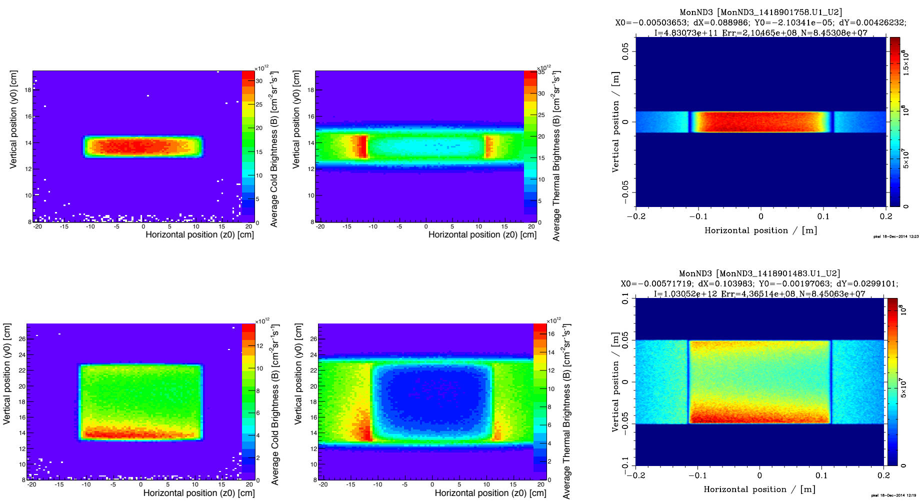


Figure 4: Top row: Emission profile at the moderator face, 1.5 cm tall moderator. Left and mid is MCNP, right is McStas. Bottom row: Emission profile at the moderator face, 10 cm tall moderator. Left and mid is MCNP, right is McStas.

TDR brilliance

Even though it may be very confusing, the best estimate for the TDR performance is the “2013” brilliance rather than the “TDR” brilliance, the reason being that the latter does not include an updated thermal brilliance.

On the other hand, the parameterisation does not allow for a 12 cm high moderator, and the cold moderator performance is also slightly improved from the official TDR moderators. A 10 cm moderator is described below.

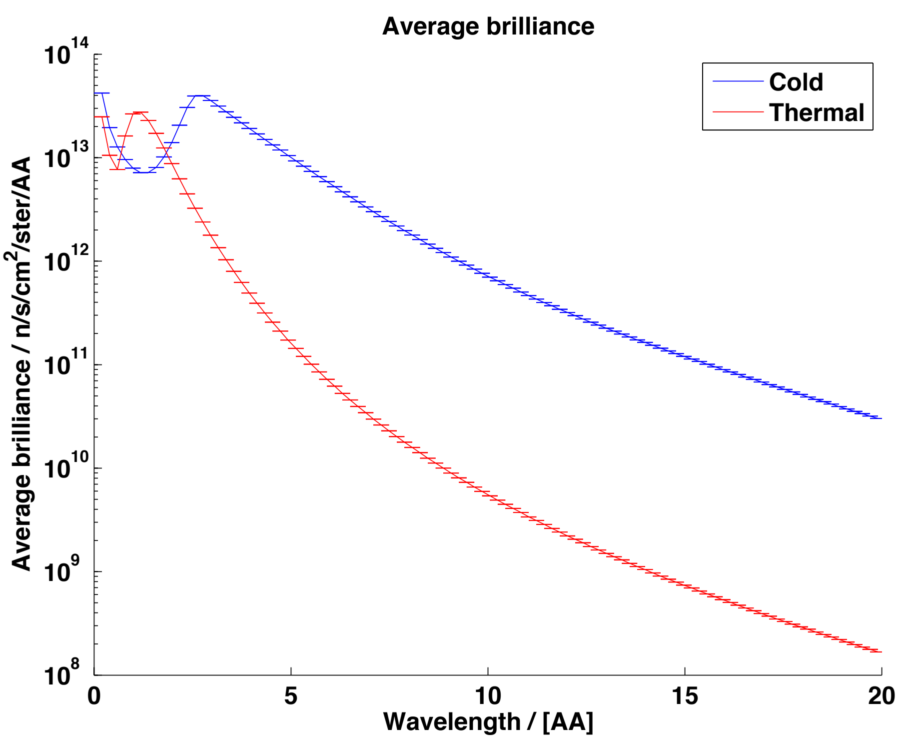
The 10x10 cm2 volume moderator may be modelled using this set of parameters:

```
COMPONENT Source = ESS_moderator(dist=2,
             focus_xw=guidewidth, focus_yh=guideheight,
             Lmin=lambdamin, Lmax=lambdamax, cold_frac=0.5,
             sourcedef=“2013”, yheight_c=0.10, yheight_t=0.10,
             xwidth_c=0.10, xwidth_t=0.10)
AT (0, 0, 0) RELATIVE Origin
```

The following parameters can be adjusted from their defaults:

- 0 < cold_frac < 1 defines the fraction of statistics emitted from the cold source
- 0 < isleft < 1 defines the fraction of the thermal statistics which is emitted from the “left” or upstream wrt. proton beam thermal wing
- yheight_c and yheight_t are used to define the height of the pancake-moderator. The brilliance varies with this height.

McStas simulation output for the thermal and cold TDR moderator respectively can be seen below



Work is under way to include the next set of optimised sources in McStas, they should become available with McStas 2.2 during spring 2015.