ESS Thermal Powder Diffractometer

We will here build a simple time-of-flight powder diffractometer. The basic philosophy is that a polychromatic beam is sent on to the sample and the diffracted neutrons are counted in time-of-flight detectors covering a large part of the solid angle. To interpret the data, one applies the basic time-of-flight equation

$$t = \alpha \lambda L, \tag{1}$$

where $\alpha = m_{\mathrm{n}}/h \approx 252.7\,\mu\mathrm{s/m/Å}$. One then assumes that all detected neutrons are scattered elastically, whence λ can be calculated. In turn, the scattering vector q can be found from 2θ, the scattering angle found from the detector position:

$$q = 2k_{\mathrm{i}} \sin(\theta) = \frac{4\pi}{\lambda} \sin(\theta). \tag{2}$$

1 Exercise 1: Source, sample and detector

1.1 The ESS moderator

ESS is a long-pulsed source, with the most important parameter being the pulse length, here called d, and the repetition frequency, $f = 1/T$. Make a simple instrument using the ESS thermal moderator which emits neutrons directly into a time-of-flight detector, simulating a typical thermal wavelength range.

Use the standard parameters for a thermal source. Simulate only one pulse and use $d = 2.8$ ms, $f = 14$ Hz, and a moderator size of 12x12 cm^2.

1. Place one time-of-flight monitor directly at the moderator, one at 6 m distance, and one at 149.9 m distance. The monitors should have the same size as the moderator, and the moderator should focus on the 149.9 m monitor. Perform the simulation. Adjust the timelimits to see the full pulse.

2. Next, place wavelength sensitive TOF monitors, at these three positions and repeat the simulations. Notice how a given time channel contains a sharper wavelength information at the long distance.

3. Third, the ESS had planned to use $d = 2.0$ ms, $f = 20$ Hz at a time: This should have the same time-integrated flux as the current setting, given constant peak flux. Confirm that by simulations of the full wavelength band.

1.2 Frame overlap

Go back to the first settings of d and f and turn on a second pulse of the moderator. Notice that some time channels at the 149.9 m monitor has ambigious wavelength information. This is known as frame overlap. To avoid this, the wavelength band, $\Delta\lambda$, of the neutrons must be limited by the frame overlap conditions, *i.e.* neutrons from two following pulses (time T apart) must not mix. This gives rise to $T \geq \Delta t = \alpha \Delta\lambda L$, or

$$\Delta\lambda \leq \frac{T}{\alpha L}. \qquad (3)$$

In reality, this is performed by frame overlap choppers at distances of 10-50 m from the moderator. In the further simulations, you will merely limit the simulated band.

1. Test by simulations the width of the possible wavelength band which avoids frame overlap.

1.3 Powder sample

Let us go back to simulating just one pulse and postpone the simulation of the guide system. We place a 6 mm diameter sample at 150.0 m distance from the source. Use a powder sample. For time-of-flight detector, we use a cylinder of 2 m radius and 20 cm height.

1. Perform the simulation and see how the scattered neutrons display a band in the (t, θ) plot. You may like to place a beamstop, *e.g.* 1 m after the sample to avoid the direct beam.

2 Exercise 2: Guides and Choppers

2.1 Neutron guides

So far we just have a sample at 150 m from the source. Now we want to increase the intensity on the sample by using neutron guides:

1. Put a 0.3cm x 3 cm slit directly in front of the sample. Note the spectrum of neutrons reaching the sample as well as the number of simulated trajectories and the neutron intensity on the sample. Now replace the 150 m of empty space between source and sample by 2 m space followed by a 147.9 m long straight guide with 12x12 cm^2 cross-section and $m = 2$ coating (leave 10 cm between guide end and sample). In the source, focus the beam on the guide entrance and simulate. Compare number of trajectories and intensity. Look at the spatial extension of the beam at the sample position (before the slit) and at the divergence.

2. Replace the last 5 m of guide by a linear guide converging from wxh of 12cm x 12cm to 1 cm x 4 cm, compare.

3. Change coating to $m = 6$ in focusing part, compare spectrum and intensity

2.2 Waveband definition chopper

Now we want to remove the artificial waveband restriction in the simulation and select our desired waveband by choppers. To select a certain waveband $[\lambda_{min}, \lambda_{max}]$, we want the chopper to open when the fast neutrons (λ_{min}) from the end of the pulse reach the chopper position, and to close when the slow neutrons (λ_{max}) from the beginning of the pulse arrive.

1. Remove the wavelength restriction in the source and select a waveband between 0.7 Å and 2.5 Å by a chopper at 6.5 m. It should have a radius of 35 cm, spin with 5 times the source frequency and have an angular opening of 2.5° at an offset of 102°. Select the window height such that it matches the guide. Simulate and test if this selects the right waveband. (Divide the guide at 6.5 m to place the chopper. Remove the curvature if you have one so you can build each guide part of one piece to save simulation time.)

2. add a counter-rotating chopper and look at the selected tine and waveband.

If you still have time, you can expand the wavelength band to get frame overlap when using more than one pulse, and remove it with a frame overlap chopper. Remove the second chopper of the double-rotating ones for this to save simulation time.
You could also try focusing the neutron beam into the chopper window with the first 4.5 m of guide, use an elliptic guide shape and/or kink the guide. Note that there will also be an optional exercise about advanced guide shapes tomorrow.