The chopper parameters

By "chopper parameters" we mean the wavelength, the master speed, the frame overlap speed ratio denominator (m), the resolution mode, and the histogram delay time. These parameters determine the speeds, phases and pickup pulse delays for the seven choppers.

In this document we shall discuss the meanings of the chopper parameters. (For more detailed explanations please talk to your local contact). We shall also offer advice on how to choose the chopper parameters.

The wavelength λ is self-evident. A neutron with wavelength λ (in Å) has an energy E (in meV) given by $E \approx 82/\lambda^2$. Furthermore its speed v (in mm/μs) is approximately 4/ λ. Since the DCS sample-detector distance is about 4 m, a neutron with wavelength λ takes the approximate time T=1000 λ (μs) to travel that distance.

In normal operation six of the seven choppers run at the so-called master speed ω_0. In principle ω_0 can take any value from 1200 to 20,000 rpm (20 to 333.33 Hz), but in practice we almost always operate with a master speed of 20,000 rpm. The remaining chopper (chopper 5, choppers being numbered from North to South, i.e. chopper 1 being closest to the sample) is called the "frame overlap chopper". It is operated at the same speed $\omega_{FO} = \omega_0$ or else at a lower speed, either $\omega_{FO} = \omega_0 / m$ or $\omega_{FO} = \omega_0 (m-1)/m$, where the frame overlap speed ratio denominator m is a small integer greater than 1. The corresponding frequency of pulses at the sample, ω_S, is ω_0 if $\omega_{FO} = \omega_0$, otherwise ω_0 / m if $\omega_{FO} = \omega_0 / m$ or $\omega_{FO} = \omega_0 (m-1)/m$. The period of a chopper turning at 20,000 rpm (333.33 Hz) is 3000 μs.

Each of the pulsing and monochromating disks has three slots with different widths. By suitably phasing the choppers we can choose among three distinct intensity/resolution conditions without having to change the wavelength or the speed of the choppers. These three conditions, or modes, are known as **"low resolution"**, **"medium resolution"** and **"high resolution"**. (We almost never use the "high resolution" mode because there is very little intensity.)

The histogram delay time, generally called "tsdmin" (minimum time from sample to detector), is the time of flight from sample to detector corresponding to the start of the first histogram time channel. Its significance will hopefully become apparent in the following discussion, "Deciding the chopper parameters".

Deciding the chopper parameters

As previously stated, the “chopper parameters" are the incident wavelength λ, the master speed ω_0, the speed ratio denominator m, the resolution mode r, and the histogram delay time tsdmin. In what follows we shall assume that the master speed ω_0 is 20,000 rpm. We shall also assume that all time channels have the same width, this being the default situation. (By default the time channel width is T/1000 where T is the time between pulses at the sample.) We are left with λ, m, r, and tsdmin.

Important considerations in choosing the chopper parameters include

- intensity at the sample,
- resolution in wave vector transfer Q and energy transfer $\hbar\omega$,
- ranges in Q and $\hbar\omega$,
- the scattering properties, temperature, size and shape of the sample
- Bragg peak contamination
- known spurions (ask your local contact).

Go to the DCS home page and click on the "Performance" link to see the total intensity in the beam as a function of wavelength, $I_r(\lambda)$ for the three DCS resolution modes. Since the beam intensity is essentially independent of height but varies across the width of the guide, the intensity of neutrons that strike the sample may be written as

$$I_S = I_r(\lambda)\frac{H}{100}f(W)\frac{1}{m}$$

where H and W are the height and width of the sample in mm and f(W) is the fractional intensity in the central W mm of the beam:

$$f(W) = \int_{-W/2}^{W/2} i(x)dx \bigg/ \int_{-\infty}^{\infty} i(x)dx$$

(Plots of the functions i(x) and f(W) are not currently available.)

In order to understand how to choose m we need to explain the problem of frame overlap. Basically frame overlap occurs when neutrons from a given pulse get mixed up with neutrons from the succeeding pulse. Whenever there is frame overlap there is a problem because the energy transfer associated with an event cannot be unambiguously determined. The purpose of the frame overlap chopper is to reduce the frequency of pulses at the sample so that frame overlap is insignificant. (It never goes away completely.)

The choice of m is critical since the intensity at the sample is proportional to 1/m. If m is too small the experimental data may be unusable because of frame overlap. On the other hand m can be unnecessarily large in which case intensity is sacrificed for no good reason. Since it can be argued that for a given experiment the most reasonable choice of m is proportional to λ, a plot of $I_r(\lambda)/\lambda$ could be useful.

In deciding the value of m, the important thing to remember is that m is determined by the scattering properties of the sample. What matters is what the sample does with the neutrons rather than simply what it does that is of interest to the user.

To develop a feel for the choice of m and the dependence of m on λ, consider first a *hypothetical* sample that only scatters neutrons elastically. In that case the distribution of arrival times at the detectors is much narrower than the minimum chopper period. Hence m=1 for all wavelengths since frame overlap cannot occur.

Consider next a sample that only scatters neutrons elastically or with neutron energy loss; this situation approximately represents that of a cold sample. The scattered neutrons have final energies E_f from almost zero to the incident energy E_0 so possible flight times from sample to detector, t_{SD}, vary from t_{el}, the time of flight from sample to detector for elastically scattered neutrons, to very large values. Since t_{SD} varies as $E_f^{-1/2}$ and $dt_{SD} \propto E_f^{-3/2} dE_f$, relatively narrow features at very small final energies are greatly broadened and reduced in intensity in the time domain. Hence the time-of-flight distribution becomes virtually flat, and very weak, as E_f approaches E_0. For this reason it is typically argued that one need only consider final energies down to a minimum value $E_{min} = E_0 / f$ where f is something like 3 or 4. This means that times of interest range from $t_{min} = t_{el}$ to $t_{max} = t_{el}\sqrt{f}$. Roughly speaking $t_{el}(\mu s) = 1000\lambda[Å]$ since a 4 Å neutron travels at about 1 mm/μs and the distance from sample to detector is roughly 4000 mm. Hence $m \approx (t_{max} - t_{min}) / T = (\sqrt{f} - 1)\lambda[Å]/3$. Thus if $f = 3$, $m \approx 0.24\lambda[Å]$. If $f = 4$, $m \approx 0.33\lambda[Å]$.

Now consider a warm, e.g. room temperature, sample that scatters neutrons elastically and inelastically with both neutron energy loss and neutron energy gain. To simplify the discussion we assume that all final energies are possible so that times of interest range from $t_{min} = 0$ to $t_{max} = t_{el}\sqrt{f}$ and $m \approx (t_{max} - t_{min}) / T = \sqrt{f}\,\lambda[Å]/3$. In this case if $f = 3$ $m \approx 0.58\lambda[Å]$, and if $f = 4$ $m \approx 0.67\lambda[Å]$.

An initial rule of thumb is that for warm samples m should be roughly λ/2 whereas for cold samples m should be roughly λ/3.

To illustrate the choices of m and tsdmin, consider a measurement of room temperature water using 7.5Å neutrons. Panel (a) (Sorry, not yet available) shows the data summed over scattering angle, plotted as a function of t_{SD}. The master speed was 20,000 rpm and the speed ratio denominator m was 4 so the time between pulses was 12,000 μs; tsdmin was chosen to be 500 μs. Thus t_{min}= 500 μs and t_{max} = 12,500 μs, i.e. E_f ranges from ≈336 meV to ≈0.92 meV. To the extent that no scattering is expected with energy transfers exceeding 300 meV, and the plot is essentially flat at long times, m and tsdmin were well chosen. Panel (b) (Sorry, not yet available) shows the effect of changing tsdmin to 3,500 μs. The plot has been wrapped around the y axis and no information has been lost, but the scattered energy no longer decreases monotonically with increasing time channel; the standard DCS data reduction software would need to be modified to handle this type of situation. In general it is not possible to predict the consequences of changing m, unless the original m is an integer multiple of the modified m. In the present case we can predict with confidence what would happen if m were changed from 4 to 2. The time between pulses at the sample would become 6,000 μs so that the second half of the spectrum would be superimposed on the first half. The two components are shown in panel (c) (Sorry, not yet available) and their sum is shown in panel (d) (Sorry, not yet available). Panel (d) represents what would be measured if m were 2 and tsdmin were 3,500 μs. Clearly the data cannot be analyzed, even though the inelastic scattering is of no interest to the user. The inelastic scattering has badly contaminated the quasielastic scattering.

Go to the DCS home page and click on the "Performance" link to see the elastic energy resolution and the elastic Q range of DCS as a function of wavelength. Note that both the energy resolution and the Q resolution improve with increasing λ (decreasing E_0). The elastic Q range decreases with increasing λ. The available energy transfer range in neutron energy loss also decreases with increasing λ.