Data reduction for tof SANS

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With time of flight SANS becoming increasingly popular, even at reactor sources, it is worth reviewing data reduction methods. Following the early work of Seeger, Hjelm & Pynn [1] the method used at ISIS [2] to extract tof data at a particular Q is:

$$I(Q) = \frac{\partial \Sigma(Q)}{\partial \Omega} = \frac{A_H \sum_{R,\lambda \subset Q} C(R,\lambda)}{A_S t \sum_{R,\lambda \subset Q} M(\lambda) T(\lambda) D(\lambda) \Omega(R)} \qquad (1)$$

The numerator sums neutron counts C(R,λ) over all radii and wavelengths contributing to a particular value of Q, so has a clear Poisson error. The denominator includes three wavelength dependent corrections: for incident monitor spectrum M(λ), measured sample transmission T(λ) and relative detector efficiency D(λ), whilst Ω(R) is a detector pixel solid angle. Function D(λ), the "direct beam" may be measured by placing a mask of area A_H at the sample, and removing the beam stop. The scattering volume of the sample is the beam area A_S times sample thickness t.

The simplicity of (1) masks a number of important details when it comes to practical implementation. In particular we have to take care that the transmission T(λ) gives the desired scattering probability, for which it must optimally include the SANS signal but exclude background. Whilst at fixed wavelength an erroneous transmission will simply be a scalar error, in tof this might also lead to a subtle change to the shape of the cross-section. Since Q resolution varies inversely with wavelength equation (1) will not give the optimal resolution due to the relatively large fraction of shorter wavelengths in the usual incident spectrum. Thus, at the expense of counting statistics, it may be helpful to remove short wavelengths close to the beam stop for some types of science.

These and other related matters will be considered in the presentation.

[1] Seeger, P.A., Hjelm Jr, R.P., Journal of Applied Crystallography, 24, 1991, 467-478.
[2] Heenan, R.K., Penfold, J., King, S.M., Journal of Applied Crystallography, 30, 1997, 1140-1147.