Time of flight SANS data Reduction

(nothing really new here, but perhaps presented in unfamiliar ways)

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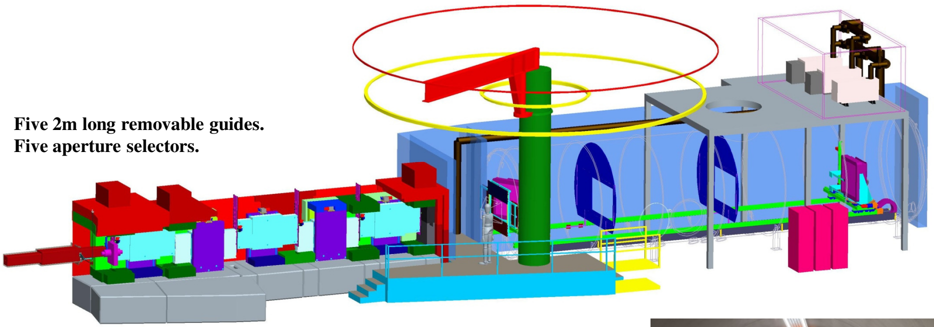
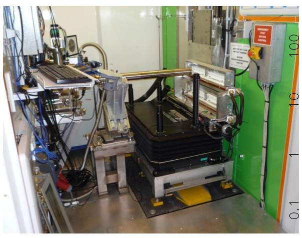
SANS2d ***Collimation L_1 = 2 to 12 m, Sample to detector L_2 = 3.5 to 12 m,***

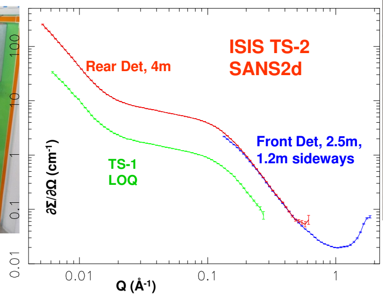
Q_{min}~ 0.0015 Å^{-1}, λ = 1.75 to 12.5 Å (12m) or 16.5 Å (4m) by time of flight, Q_{max}~ 2 Å^{-1}

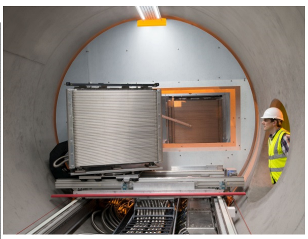
Five 2m long removable guides.
Five aperture selectors.





Sample position 19m from moderator, mezzanine 1m below beam height.





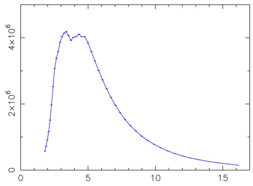
Two 1m square detectors in a 13m long, 3.25m diameter vacuum tank.

We like to obtain absolute SANS scattering probability, e.g. for dilute particle in a matrix:

$$\frac{\partial \Sigma(Q)}{\partial \Omega} = N.V^2 F^2(Q)(\rho_P - \rho_M)^2$$

Ought to obtain the same result for "mirror image" systems, e.g. D particle in H solvent (low transmission, "high incoherent background") as for H particle in D solvent (high transmission, low background).

Data reduction needs to work well over a wide range of wavelengths.



Need to allow for "strong scattering" – at the longest wavelengths a large fraction of the beam may be scattered.

For this we need the scattering probability for our particles, in the absence of any other process that may be going on. (i.e. ignoring background, wide angle scatter, adsorption and inelastic scattering - most of which we don't have a good theoretical description of.)

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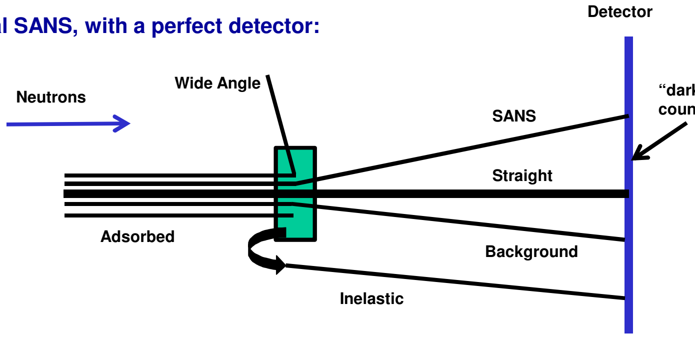
Ideal SANS, with a perfect detector:



$$\frac{\partial \Sigma_{SANS}(Q)}{\partial \Omega} = \frac{SANS(Q)}{\int Straight + \int SANS}$$

= Probability in the absence of any other process

$$= \frac{Counts(Q) - Background(Q) - Inelastic(Q) - Dark(Q) - Straight(Q)}{\int Straight + \int SANS}$$

Note – no transmission measurement is needed. Alas present detectors do not have the dynamic range and spatial uniformity required.

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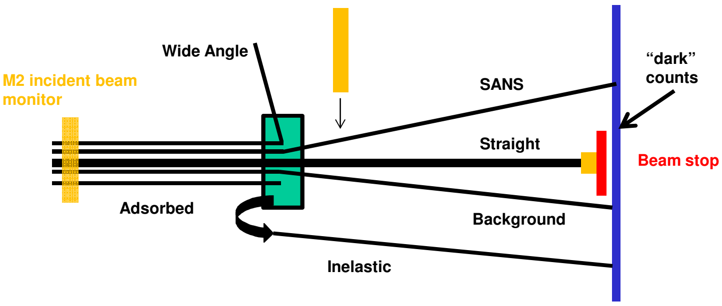
Real SANS:



Monitors M2, M3 and M4 may not sample the entire beam, nor sample it uniformly.

Even "beam stop out" transmissions may not fully sample the straight through beam (e.g. some of it may pass through a gap between gas tubes).

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For coherent SANS signal:

$$Counts(R,\lambda) = I_0(\lambda)\frac{\partial\Sigma(Q)}{\partial\omega}\Omega(R)t.T(\lambda)\eta(\lambda)$$

Incident flux: $I_0(\lambda) = \frac{M(\lambda)}{\eta_M(\lambda)}$

Wavelength λ is proportional to arrival time at detector. Need ratio of main detector efficiency compared to monitor. e.g. Remove beam stop and put a small hole A_H at the sample to record:

$$D(\lambda) = \frac{C_H(\lambda)}{M_H(\lambda)} = \frac{\eta(\lambda)}{\eta_M(\lambda)}\frac{A_H}{A_S}$$

Rearranging:

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

R – radius on detector
t – sample thickness
T – transmission
η – detector efficiency

M – incident beam monitor
C – neutron counts
Ω – solid angle
A – beam area
$V_{sam} = A_s t$ – sample volume

Proper statistics are not obtained by "averaging the reduced data at each wavelength"
Sum the counts in a time and space "Q bin".

P.A.Seeger & R.P.Hjelm J.Appl.Cryst. 24(1991)467-478

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In reality, use standard sample (a coherent scatterer, not H_2O) for "Scale" factor.

$$I(Q) = \frac{Scale}{V_{SAM}} \frac{\sum_{R,\lambda \subset Q} C(R,\lambda)}{\sum_{R,\lambda \subset Q} M(\lambda) T(\lambda) D(\lambda) \Omega(R)}$$

- **Three λ dependent corrections:** Incident spectrum M(λ),
  Detector efficiency ratio D(λ)
  Experimentally measured transmission T(λ) relative to an *empty* beam.
- **At ISIS we empirically adjust D(λ) using standard sample, as it varies slightly with L_1 and collimation since the monitor does not see exactly the same spectrum as the sample. Monitor allows for changes in moderator temperature or filling.**
- **A reactor source moderator may be stable enough for M(λ) to become a scalar for exposure time and thus D(λ) just the beam stop out empty beam, which may then cancel with the denominator of T(λ). [Assuming attenuator used for "beam stop out" is same factor at all λ.]**
- **Assume η(λ) is same over whole detector, incorporate flood source measured scalar efficiency per pixel into Ω(R).**

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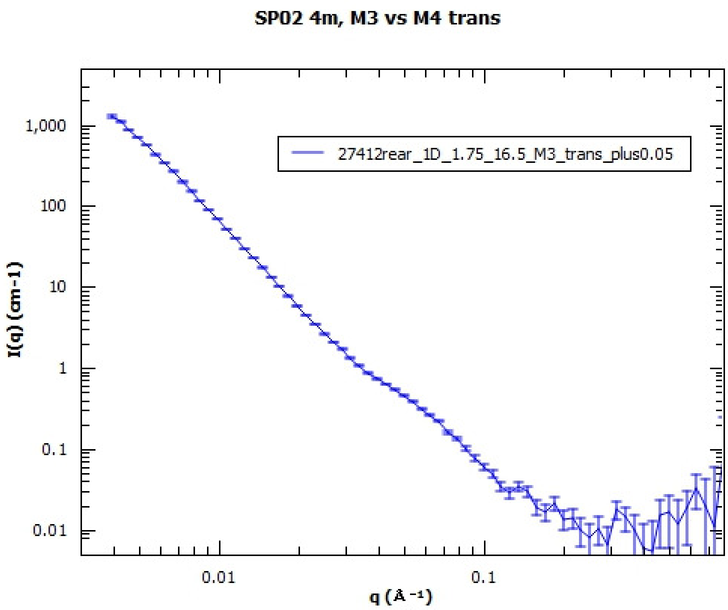

Recent iron oxide solution in H_2O (SANS2d)

Rear detector $L_1=L_2=4m$

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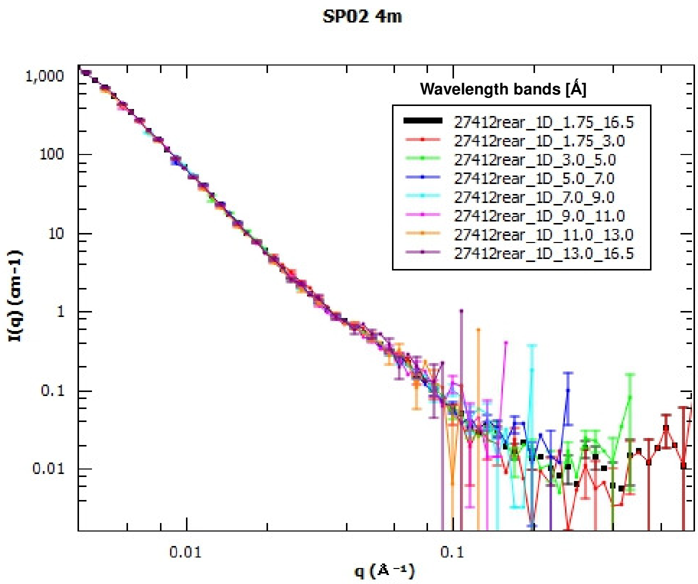
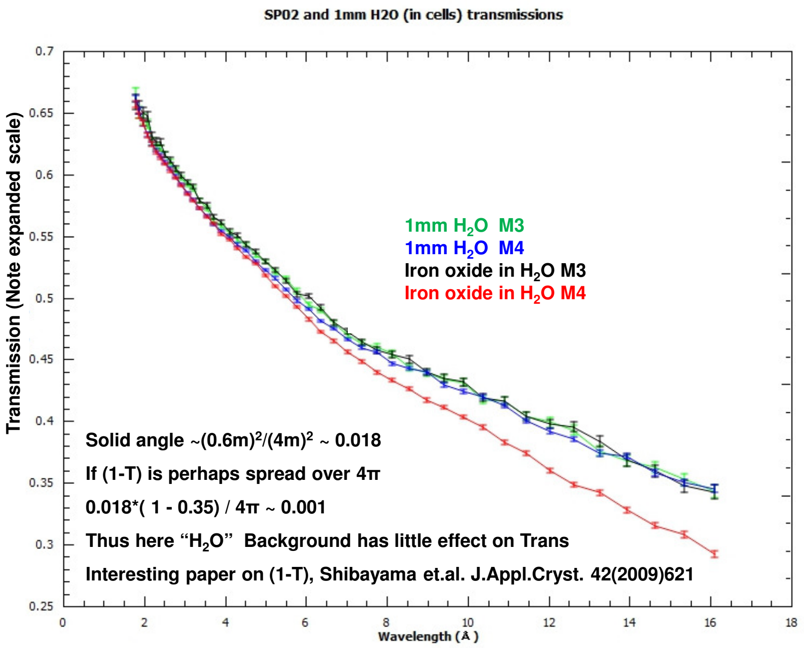
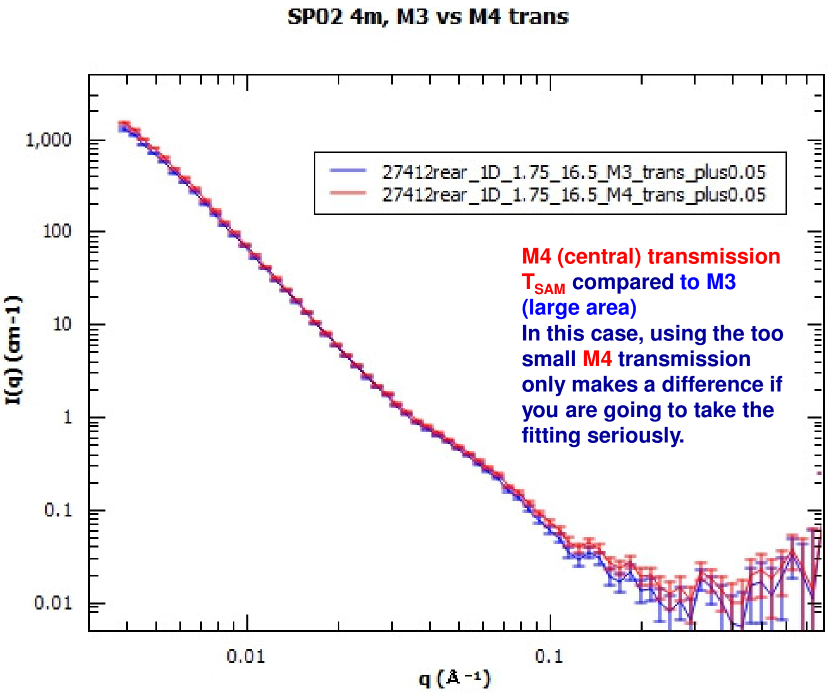
Wavelength overlap plots are a key check!
Q resolution (and any multiple scatter from strong scatterers) varies with λ.

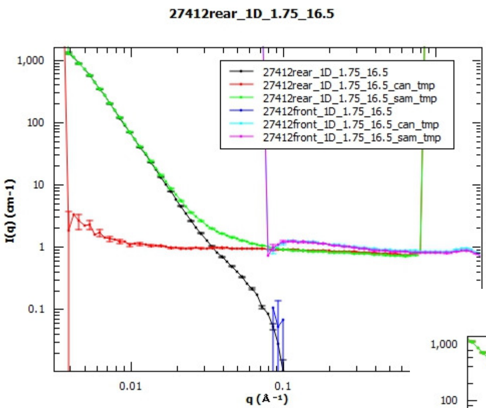


Recent iron oxide solution in H_2O (SANS2d)

Rear detector L_1=L_2=4m



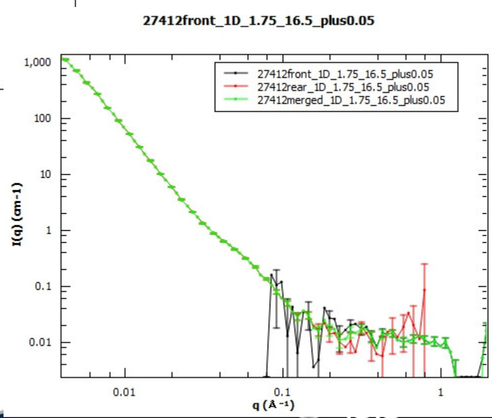


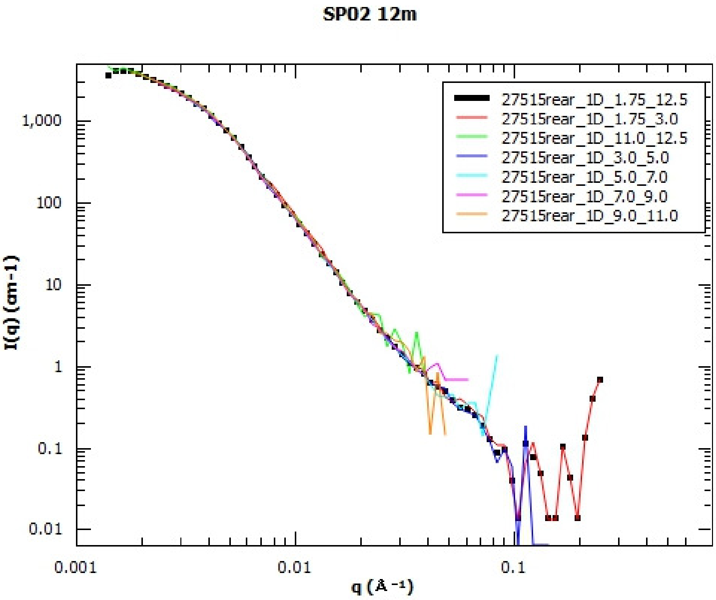


Recent iron oxide solution in H_2O (SANS2d)

ISAM and ICAN subtraction for Rear (4m, 0.25m sideways) and Front (1.8m, -1m sideways, rotated 25°)

Merged data below.

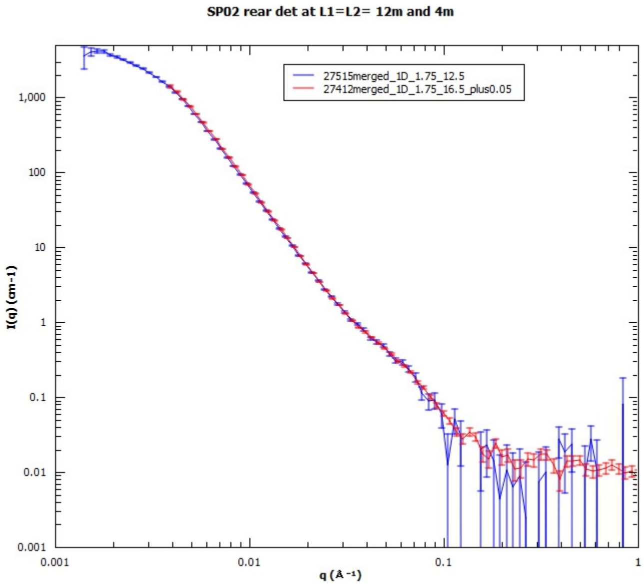




Recent iron oxide solution in H_2O (SANS2d)

Rear detector $L_1=L_2=12m$

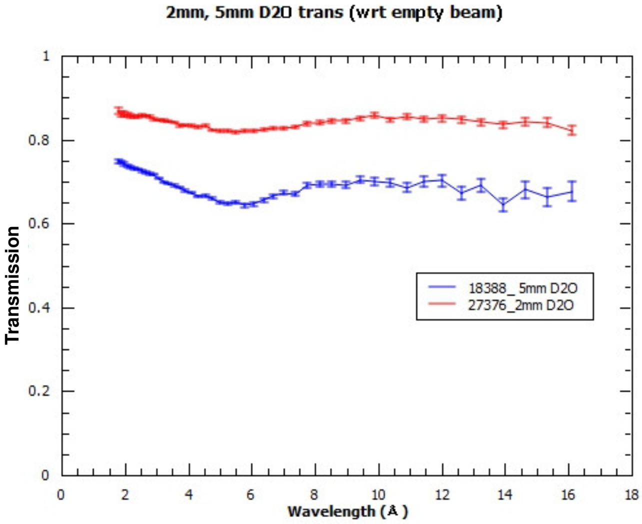
The >5% scatter at smallest Q does not show serious multiple scatter, so the downturn here is genuine.



Recent iron oxide solution in H_2O (SANS2d)

Compare merged data from 4m and 12m runs.

Shoulder at ~0.06 and downturn at smallest Q are genuine.



Some "unexpected" features in transmissions

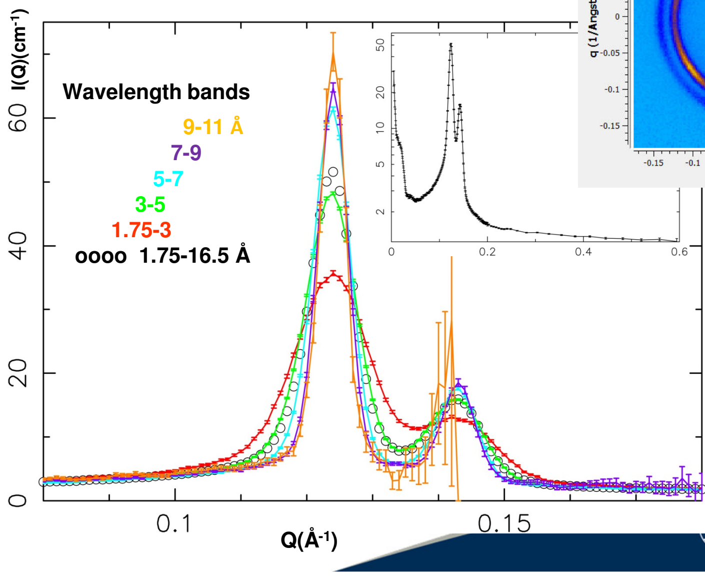
"Overlap" plots generally good – but can we do better?

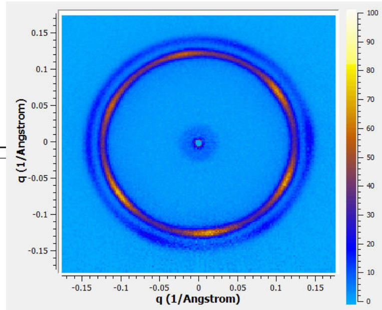
- **Need all the effects at "few %" level, e.g. angle dependent T(λ), detector path length & parallax, detector efficiency.**
- **Transmission T(λ) is key. Actually to some extent we don't actually need to calculate T(λ), but it is an extremely useful diagnostic.**
- **T(λ) should include the SANS and straight through beam, but not the Background & Inelastic. Fortunately H_2O scatter is not usually a significant effect on the transmission.**
- **M4 beam stop detector transmissions are good (possibly better?) for weak scatter.**
- **M3 transmissions are better for strong scatter, as they include most of the SANS.**
- **Beam stop out transmissions as a function of detector radius are a useful diagnostic in conjunction with "overlap checks".**

Q resolution varies inversely with λ

- can remove shorter wavelengths to sharpen peaks.

[Cubic phase with silica particles, W.Briscoe (Bristol)]





DETOUR – the traditional reactor method is the same …

I_{SAM} = raw counts of sample in can (includes $T_S T_{CAN}$)

I'_S = raw counts due to sample alone (includes T_S)

I_{CAN} = raw counts can (includes T_{CAN})

T_S = sample transmission, by measuring (sample in can)/(empty can)

$T_{SAM} = T_S.T_{CAN}$ = sample in can transmission relative to empty beam

"CAN" here may also be solvent in a cell.

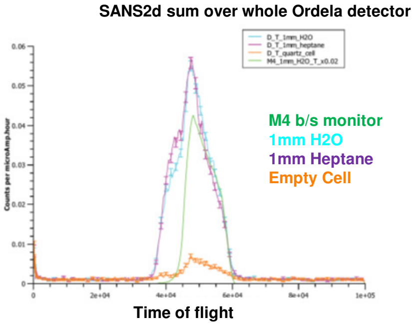
Assume $$I_{SAM} = I'_S T_{CAN} + I_{CAN} T_S$$

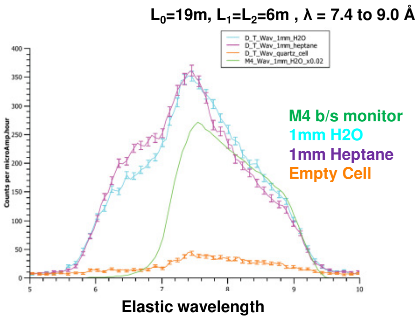
then $$I'_S = \frac{1}{T_{CAN}}\left(I_{SAM} - T_S I_{CAN}\right)$$

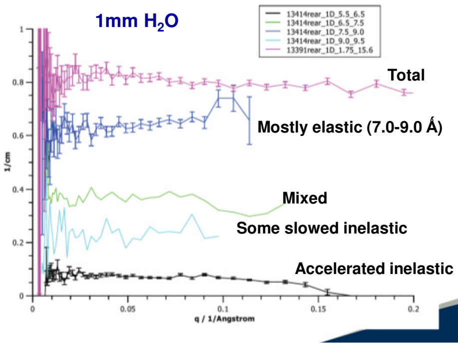
Some reactor sources first do this, or something similar.

$$\frac{\partial\Sigma(Q)}{\partial\Omega} \propto \frac{I'_S}{T_S} = \frac{I_{SAM}}{T_S T_{CAN}} - \frac{I_{CAN}}{T_{CAN}} = \frac{I_{SAM}}{T_{SAM}} - \frac{I_{CAN}}{T_{CAN}}$$

ISIS does this, with symmetrical reduction for Sample & Can, and all transmissions relative to empty beam.







Using our chopper as a "monochromator", inelastic scatter is interesting but fortunately the accelerated neutrons usually appear under stronger signals at shorter wavelengths.

Effects are larger when L_2 is large compared to L_0+L_1, e.g. LOQ and LQD.

Also see: Do, Heller et.al. Nucl Instr Meths A 737(2014)42

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TIME OF FLIGHT SANS DATA REDUCTION

- **Conceptually simple, in detail a bit tricky.**
- **Many samples scatter significant fractions of the beam.**
- **Future projects: Though tof SANS does not always collect to good statistics at every single wavelength, reduction software should be able to flag issues such as very low transmission or multiple scattering. In tof we should be able to deconvolute modest multiple scattering.**
- **Wavelength overlap can be improved further still with attention to all the "few % effects". (Except at extremes of Q tof averages over a large detector area.)**
- **Software www.mantidproject.org – ask me for a demo later.**

Many thanks to: Phil Seeger for the initial method;
the Mantid team for software implementation and being patient with all my requests;
Charles Dewhurst & Isabelle Grillo for letting me play on D33.

ISIS