Improving the accuracy of time of flight neutron total scattering data and analysis

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Total scattering and pair-distribution function (PDF) methods allow for detailed study of local atomic order and disorder, including materials for which Rietveld refinements are not traditionally possible (amorphous materials, liquids, glasses, nanoparticles). With the advent of modern neutron time of flight (TOF) instrumentation, total scattering studies are capable of producing PDFs with ranges upwards of 100 - 200 Angstroms, a regime of great interest in complex materials. Despite this, the refinement and subsequent analysis of data is often limited by confounding factors that are not rigorously accounted for in conventional analysis programs. We have explicitly explored the effects of resolution, peak-shape, peak-asymmetry, and related factors in neutron TOF data as they relate to real-space PDF analysis through simulation. In addition to the simulated studies, we will present three case studies of neutron TOF powder diffraction instruments, where the interplay of these effects can be observed. Based on both the simulated and real-world case studies, we present best practices for analysis of data from modern neutron TOF total scattering instruments, demonstrating marked improvement in quality of fits at all length scales.