

Angle-Dependent Absorption Correction for Reliable Absolute-Scale SAXS and SWAXS in Kratky-Type Geometry

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Reliable absolute-scale SAXS and SWAXS analysis requires an accurate correction for X-ray absorption by the sample. In line-collimated Kratky-type instruments with cylindrical capillaries, this is commonly performed using a scalar transmission factor derived from the measured attenuated primary beam [1]. While this approach is often adequate for sample series with similar X-ray absorption, it can become unreliable when the sample, reference solvent, and empty capillary exhibit substantially different X-ray absorption. This becomes particularly evident in extreme cases in the wide-angle region of SWAXS, where background subtraction may even yield unphysical scattering results [2]. Here we introduce a numerical angle-dependent absorption correction for SAXS and SWAXS in a realistic Kratky-type geometry. The method combines tabulated attenuation coefficients with an explicit description of the experiment, including the constrained scattering volume, measured primary-beam profiles, self-absorption of the scattered radiation, and attenuation in the quartz capillary wall. It therefore provides a physically consistent alternative to conventional experimental scalar transmission correction, with direct relevance for reliable background subtraction and absolute-scale calibration. The performance of the correction is assessed by comparing corrected experimental SWAXS data with theoretical scattering intensities calculated for the same systems using the complemented system approach [3–5]. The numerical correction yields markedly improved agreement, supporting its use for quantitative SWAXS analysis. A simplified Beer–Lambert-type scalar correction can still give similar results in the small-angle range, whereas the comprehensive numerical treatment is required for physically consistent angle-dependent SWAXS correction. The present approach thus offers a practical correction procedure for line-collimated SAXS/SWAXS experiments, especially when measurements with substantially different absorption must be combined within the same data-reduction and absolute-scaling procedure.

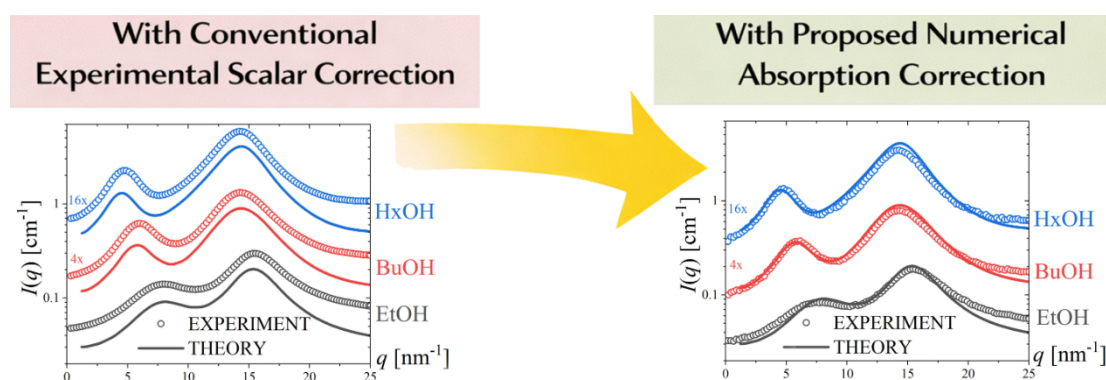


Figure: Experimental (circles) and theoretical (lines) SWAXS profiles for EtOH, BuOH, and HxOH. Left: conventional scalar correction shows major deviations. Right: proposed numerical absorption correction improves agreement.

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