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Interpreting SAXS spectra of non-spherical nonane-water nanodroplets using a new particle form factor[1] ABDALLA OBEIDAT, FAWAZ HRAHSHEH, GERALD WILEMSKI, Missouri University of Science and Technology, HARSHAD PATHAK, BARBARA WYSLOUZIL, The Ohio State University
— The structure of nanodroplets plays a critical role in many natural phenomena involving atmospheric nucleation and aerosol formation. Here, we review our theoretical efforts to interpret experimental measurements of small angle x-ray scattering (SAXS) from nonane/water nanodroplets formed in supersonic nozzles. We simulated nonane/water nanodroplets using classical molecular dynamics (MD) and found that they have a nonspherical Russian-Doll (RD) structure consisting of a roughly spherical water droplet partially wetted by a large nonane lens. We have developed an exact analytical expression for the particle form factor P(q) of a lens-on-sphere droplet with sharp interfaces and uniform lens and sphere densities for use in fitting the experimental data. The model was validated by comparing it with exact results for P(q) based on the MD simulations. Excellent agreement was found. The fits of the measured SAXS spectra generated with this model are good and generally better than those based on simpler structural models, but the resulting particle size distributions do not produce mass balance for either water or nonane. Further work is needed to resolve this discrepancy.

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