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Validation of pore size distribution from a new GCMC kernel based on a slit-pore model with carbon surface heterogeneity

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For porous carbons, which typically have hierarchical structures, the pore size distribution (PSD) is one of the most important characteristics and is currently evaluated by using kernel fitting methods represented by non-local density functional theory. Herein, we present new kernels for N2 and Ar adsorption at 77 K and 87 K, respectively, derived from Monte Carlo (MC) simulations based on a carbon slit-pore model that considers energetic heterogeneity due to surface roughness. The model consists of a locally scaled Lennard–Jones (LJ) 10-4 potential and Steele's 10-4-3 potential, and the scaling factors of the LJ 10-4 potential are assumed to follow a normal distribution that mimics the adsorption behavior on real carbon black. In contrast to our previous MC kernel based on Steele's 10-4-3 potential, the local isotherms of the new kernel did not show a steep increase due to adsorption layer formation. Despite the improved fit for adsorption isotherms, PSDs obtained from the proposed kernel unfortunately show a non-negligible valley around 1 nm, which is a major artifact of the kernel fitting approach. A careful comparison of the smooth and rough surface models indicated that the definitive cause of the artifact lies not in the formation of monolayers, which was believed so far, but rather in the pore-filling behavior, which provides a major clue for constructing a completely artifact-free kernel based on molecular simulations. Finally, the PSDs of four commercial activated carbons were evaluated using the new kernel[3] and compared with our previous GCMC-based kernel[1] and QSDFT[2] in Fig.1.

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