Pore wall thickness heterogeneity on adsorption in carbons using explicit slit pore model and biased GCMC

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In model of activated carbons the pores are often assumed to be slit-shaped formed either between single, perfect graphite layer planes. X-ray diffraction studies show among other disorders, that micropores are formed between stacks of different carbon layer planes. In this study we investigate the influence on the adsorbed methane and N2 densities for different graphene layers thick which have been shown to yield significant different adsorption behavior. All layers thick studies to date was performed using the Steele 10–4–3 potential that use terms from the Fourier expansion of the sum over all the individual gas molecule carbon atom interactions. Instead Steele potential, we use graphene layers made up of discrete atoms of carbon. Explicit models have the advantage of representing the corrugation of the surface and are more appropriate to the subsequent development of virtual porous carbons models (VPC). We simulated methane (300 K) and N2 (77 K) densities through the grand canonical Monte Carlo method using the biased energy scheme in pores widths between 7 to 30 Å. We also investigate the isotherms in a model with mean number of graphene layers per wall of 1.5 and the interpore adsorbate interactions. The simulation showed that N2 presents greater sensibility to the variations in the number of layers plane in pore wall than methane. The N2 isotherms changes until approximately five layers while nitrogen changes only until 2 layers. A similar behavior occurs again for the interpore adsorbate interaction that is stronger to N2. The isotherm simulation in the model with mean graphene layers of 1.5 shown that the kind of probe-molecule associated with pore wall thickness will interfere with the pore size distribution analysis.