Theoretical isosteric heat of adsorption calculation in the Henry’s law region for carbon nanopores and nanocavities

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The isosteric heat of adsorption in the Henry's law region is calculated as a function of the pore width for carbon single wall cylindrical nanopores and spherical nanocavities. The maximum isosteric heat of adsorption is obtained for six gas molecules: argon, methane, carbon dioxide, hydrogen, helium, and nitrogen. In addition, the results for cylindrical carbon nanopores are compared with adsorption data on single-wall carbon nanotubes from the literature. We find the pore width where the isosteric heat of adsorption is a maximum for both geometries. The effect of solid-fluid parameters on the pore diameter for the maximum isosteric heat of adsorption is determined for any system described by a Lennard-Jones potential. Constant relationships between the pore diameters for the maximum isosteric heat of adsorption and the specfic solid-fluid parameters are found for cylindrical nanopores, spherical nanocavities, and parallel-wall slit-shaped pores. Surface mean curvature has a significant influence on the isosteric heat of adsorption.