223g Comparison of Adsorption of Spherical and Non-Spherical Nitrogen in Parallel Slit Pores Using Density Functional Theory: Density Profiles and Pore Size Distributions

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The diatomic nitrogen molecule is commonly used to determine pore size distributions of nanoporous adsorbents, and for this purpose it is assumed to be spherical. In this paper, first-order thermodynamic perturbation theory is combined with density functional theory to treat nitrogen as a non-spherical molecule instead of a spherical molecule. The analysis shows that the treatment of nitrogen as a non-spherical molecule affects the equilibrium density profile in parallel slit pores, with pore filling occurring at lower pressures for the non-spherical case than the spherical case. The differences become more pronounced at higher pressures and larger pore widths. These changes in the equilibrium density profile effect the pore size distribution calculated by density functional theory. We discuss the effect of treating nitrogen as a non-spherical molecule on the pore size distribution. We compare the pore size distribution calculated for non-spherical nitrogen with the pore size distributions for spherical nitrogen and argon on various activated carbons.