Critical properties of fluids in nanopores: Crossover from 3D to 2D

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Investigation of phase coexistence, adsorption, diffusion and reaction of fluids in porous materials is of much interest from both scientific and industrial point of view. In general, molecules confined within narrow pores, with pore widths of a few molecular diameters, can exhibit a wide range of physical behavior. We examine the vapor-liquid phase transition of variable square-well fluid and n-alkane under slit and cylindricall pore using grand-canonical transition matrix Monte Carlo with histogram reweighting technique. We examine the critical property shift as a function of slit width, H and pore radius R, varying from 30.0 to 1.0 molecular diameter. This investigation on various fluids indicates that the critical properties (Tc, ρc and Pc) show interesting trends under confinements of different shape and size, contrary to earlier prediction.