

THERMODYNAMICS

乙烯分子在狭缝炭孔内的毛细相变和自扩散

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摘要 The grand canonical Monte Carlo (GCMC), the canonical Monte Carlo by using equal probability perturbation, and the molecular dynamics (MD) methods were used to study the capillary phase-transition (capillary condensation and evaporation) and self-diffusion for a simple Lennard-Jones model of ethylene confined in slit carbon pores of 2.109 nm at temperatures between 141.26 K and 201.80 K. The critical point of capillary phase-transition was extrapolated by the critical power law and the law of rectilinear diameter from the capillary phase-transition data in the near critical region. The effects of temperature and fluid density on the parallel self-diffusion coefficients of ethylene molecules confined in the slit carbon pores were examined. The result showed that the parallel self-diffusion coefficients in the capillary phase transition area strongly depended on the fluids local densities in the slit carbon pores.

关键词 毛细管 相变过程 自扩散系数 乙烯 生产工艺 数值模拟 分子动力学 化工过程

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Capillary Phase-Transition and Self-Diffusion of Ethylene in the Slit Carbon Pores

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Key words capillary phase-transition; self-diffusion

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