عنوان مقاله:

Modeling of Methane Adsorption in Carbon Nanotubes by Molecular Dynamics Simulation

محل انتشار:

هفتمین کنگره ملی مهندسی شیمی (سال: 1390)

تعداد صفحات اصل مقاله: 8

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خلاصه مقاله:

Adsorbed natural gas (ANG) storage and transportation technology has recently become competitive to compressed natural gas (CNG) method. New adsorbents such as carbon nanotubes used in noncylindrical vessels have made possible to store the same capacity of gas as CNG tanks, but at much lower pressures. To modify the amount of adsorption, optimization of these porous materials is needed. The study of nanoscopic transport processes requires a molecular point of view and preferably the application of molecular dynamics (MD) simulation. So the excess gravimetric adsorption (EGA) of methane on triangular arrays of single-walled carbon nanotubes (SWNTs) consisting of (13,0), (26,0), (42,0) arrays was investigated by MD method. For every zigzag SWNT array above, the van der Waals (VDW) gap has been varied to optimize methane storage. Results indicate that the (26,0) SWNT arrays with a VDW gap of 0.85 nm is the optimal adsorbent for methane storage at room temperature

کلمات کلیدی:

Carbon Nanotubes (CNTs), Molecular Dynamics, Methane Adsorption and van der Waals Gap