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# 层柱状微孔材料吸附存储天然气的**Monte Carlo**模拟

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摘要
采用巨正则系综MonteCarlo方法模拟了天然气中主要成分甲烷在层柱状微孔材料中T=300K下的吸附存储，在模拟中层柱状微孔采用Yi等人建立的柱子均匀分布在两炭孔墙之间的模型来表征。甲烷分子采用Lennard-Jones球型分子模型，炭孔墙采用Steele的10-4-3模型，对孔宽为1.36nm的层柱微孔，模拟了四个不同孔率的层柱材料吸附甲烷的情形。得到了孔中流体的局部密度分布以及吸附等温线，对比不同孔率下甲烷的吸附量，得到了此情形吸附甲烷的较佳孔率为0.94。

关键词 层柱状 微孔 甲烷 多孔材料 油气储存 吸附 天然气 蒙特卡洛模拟 巨正则系综

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## Monte carblo simulation of natural gas adsorption storage in pillared layered material

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**Abstract** Grand canonical ensemble Monte Carlo (GCEMC) method has been used for adsorption storage of methane, the main component in natural gas, in pillared layered material at T=300 K . Pillared layered material is modeled by the approach of Yi et al . with the uniform drstribution of pillars. Methane is described as a spherical Lennard - Jones molecule, and 10-4-3 potential from Steele is used for representing the interaction between methane and a carbon wall in the GCEMC simulation. The local density profiles and the adsorption isotherms of methane adsorbed in pillared layered material with 4 various porosities in the pores of width 1.36 nm were obtained. Consequently, an optimum porosity of the pillared layered material is recommended for the adsorption storage of methane.

**Key words** MICROPOROUS METHANE POROUS MATERIALS OIL-GAS STORAGE ADSORPTION NATURAL GAS MONTE CARLO SIMULATION

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