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MFI型沸石分离CO<sub>2</sub>-N<sub>2</sub>混合物的热力学研究

Thermodynamics for the Separation of CO<sub>2</sub>-N<sub>2</sub> Mixtures by Zeolite MFI

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关键词:

CO<sub>2</sub>-N<sub>2</sub>混合物; MFI型沸石; 吸附; Monte Carlo模拟; PC-SAFT; CO<sub>2</sub>-N<sub>2</sub> Mixture; Zeolite MFI;

Adsorption Isotherms; Monte Carlo Simulation; PC-SAFT

摘要:

用Monte Carlo模拟方法, 模拟了二氧化碳(CO<sub>2</sub>)-氮气(N<sub>2</sub>)混合烟气在MFI型沸石中的吸附等温线, 分析了温度、压力及烟气组成等条件对吸附量的影响, 以及MFI型沸石对模拟烟气中CO<sub>2</sub>的吸附选择性. 用微扰链统计缔合流体理论(PC-SAFT)研究了不同温度下CO<sub>2</sub>-N<sub>2</sub>二元体系的p-x相图, 阐明了从脱吸气体中液化分离CO<sub>2</sub>所需的温度范围。

The adsorption isotherms of flue gas containing carbon dioxide (CO<sub>2</sub>) and nitrogen (N<sub>2</sub>) confined in zeolite MFI were investigated by using the Monte Carlo simulation technology. The temperature, pressure and composition dependence of the adsorption capacity of simulated flue gas was analyzed, and the selectivity of CO<sub>2</sub> was determined. The p-x diagrams for CO<sub>2</sub>-N<sub>2</sub> binary mixture at different temperatures were calculated by using PC-SAFT, and the temperatures under which CO<sub>2</sub> can be liquefied from the flue gas were illustrated.

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