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研究论文

# 温度对碳膜内氮、氧渗透分离影响的非平衡模拟

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摘要 采用双控体积巨正则系综分子动力学(DCV-GCMD)方法,
用二维狭缝代替传统的一维狭缝构建膜孔模型研究了温度对氮氧纯气体及其混合物在碳膜内的渗透特性,
探讨了氮氧分离机理. 提出了一种新的计算二元混合气体中各组分通量和分离系数的方法, 即模拟中引入迭代,
解决了前人忽略低压侧气体组成和压力影响的问题. 试验结果表明: 当氮氧以纯气体的形式分别透过碳膜时,
二者均遵循Knudsen扩散方式, 且低温下氮气具有较大的渗透性质; 而当二者以混合物的形式一起透过碳膜时,
低温下二者之间存在竞争吸附, 孔宽对气体的渗透影响显著, 尤其是膜孔较小的时候, 分子筛效应控制氮氧分离;
高温下吸附影响不显著.

关键词 碳膜 非平衡模拟 渗透 氮气 氧气

分类号

## Effect of Temperature on the Permeation and Separation of Oxygen and Nitrogen in Carbon Membranes: A Non-equilibrium Molecular Dynamics Simulation Study

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**Abstract** The effect of temperature on the permeation of oxygen, nitrogen and their binary gas mixture through carbon membranes were investigated using a dual control volume grand canonical molecular dynamics method. The two-dimensional slit was used instead of one-dimensional pore, and a novel iteration was introduced to overcome the difficulty of ignoring the effect of permeation side pressure and composition on gas transports. The results showed that both oxygen and nitrogen followed Knudsen diffusion mechanism when they permeated through carbon membranes as pure component, respectively. In this case, nitrogen had a rather higher permeability than oxygen. However, oxygen had a higher permeability than nitrogen due to competitive adsorption at low temperature when their mixture flowed through membranes. In addition, the pore width impacted the permeability strongly, especially when the pore was very small, and molecular sieving predominated the separation of oxygen/nitrogen. But at the high temperature adsorption hardly affected the separation of oxygen/nitrogen.

**Key words** carbon membrane non-equilibrium simulation permeation nitrogen oxygen

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