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H. Wang, Z.G Qu, L. Zhou

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Coupled GCMC and LBM simulation method for visualizations of CO_2/CH_4 gas separation through Cu-BTC membranes

H. Wang, Z.G Qu*, L. Zhou

MOE Key Laboratory of Thermo-Fluid Science and Engineering, School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China

* Corresponding author. Tel./Fax: +86-029-82668543; e-mail address: zgqu@mail.xjtu.edu.cn

Abstract: A fully dynamic model for mixture gas separation is built in Cu-BTC membranes. A multi-scale method that couples the lattice Boltzmann method with grand canonical Monte Carlo (GCMC) is proposed to investigate the mass transfer process of CO_2/CH_4 mixture gases in Cu-BTC membranes. The convection and diffusion in the interparticle flow field and the intraparticle diffusion and adsorption in the particle interior are simultaneously considered. The membrane morphology is reconstructed by a sphere-based simulated annealing method. The effects of membrane porosity and particle size on the mass transfer and selectivity of CO_2/CH_4 mixture gases are predicted. Results show that the selectivity of CO_2/CH_4 is mainly determined by interparticle and intraparticle mass transfer resistances. Meanwhile, the time of saturation adsorption for CO_2 and CH_4 both decrease with an increase in porosity but decreases for CO_2 and increases for CH_4 with an increase in particle size. The selectivity of CO_2/CH_4 in Cu-BTC membranes decreases with an increase in porosity and particle size. Therefore, membranes with small porosity and particle size should be utilized. Compared with the traditional binary GCMC and ISAT methods based on saturation adsorption, the proposed coupled method is closer to the physical essence of the process because it considers dynamic competitive adsorption. The present method can be helpful in the design of efficient metal−organic framework (MOF) membranes.

Key words: MOF membranes, adsorption, lattice Boltzmann method, GCMC, membrane selectivity

Nomenclature	
b	Coefficient
C	Gas concentration(mol/m^3)
D	Diffusion coefficient (m/s^2)
d	Diameter (μm)

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