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Efficient molecular simulations of binary gas mixture transport in slit nanopores

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A novel approach is suggested to simulate the gas mixture transport in slit nanopores. The proposed method is based on the modification of the dual control volume grand canonical molecular dynamics (DCV-GCMD) method. The conventional method, DCV-GCMD, describes the gas mixture transport with pre-set constant composition. Due to the selective adsorption in the nanopores, the composition of the produced gas mixture will be affected. The modified method provides the composition in the permeate side. Gas mixtures of CH4/He and CO2/CH4 are investigated in graphene, graphite, and clay slit nanopores. The results show that pore size is the dominant factor in the species separation; the solid surface roughness has pronounced effect on gas separation; the influence of average pressure is not pronounced. The effects of pore length, temperature, pressure gradient, and feed composition are also investigated.

References

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Primary author: Dr WU, Tianhao (Reservoir Engineering Research Institute (RERI))

Co-author: Prof. FIROOZABADI, Abbas (Reservoir Engineering Research Institute (RERI))

Presenter: Dr WU, Tianhao (Reservoir Engineering Research Institute (RERI))

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