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Adsorption-Induced Deformation and Its Impact on Gas Transport in Microporous Coal Matrix

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Adsorption-induced deformation in microporous coal matrix has been largely overlooked in gas transport studies, despite its significant influences on pore geometry and diffusive pathways. In this work, we employ a hybrid grand canonical Monte Carlo (GCMC) and molecular dynamics (MD) scheme under various loading conditions to capture both gas adsorption and matrix deformation behavior. Equilibrium MD simulations is then performed to quantify CH_4 and CO_2 self-diffusivity. Results show that deformation enhances adsorption, with CO_2 displaying greater uptake and volumetric strain than CH_4. A universal linear relationship among gas loading, free volume ratio, and self-diffusion coefficients holds for both rigid and flexible matrices, but with a gentler slope in flexible matrices—indicating reduced diffusion sensitivity to diminishing free volume at higher loadings. Geometrical and effective tortuosity variations reveal that strong CO_2 adsorption induces significant swelling and complex matrix rearrangements at elevated loadings, pushing geometrical tortuosity (~3.70) well beyond rigid-matrix levels (~2.49), while weak CH_4 adsorption produces milder, more uniform adjustments on matrix geometrical tortuosity (from ~2.80 down to ~2.40). Consistent drop in effective tortuosity across all cases indicates that gas motion is increasingly hindered by neighboring molecules, rather than gas-solid interactions. Overall, our findings clarify how gas adsorption, matrix deformation, and self-diffusivity co-evolve in microporous coal matrix, and provide important guidance into enhanced gas recovery and CO_2 sequestration that require accurate transport modeling in deformable media.

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References

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