Molecular Dynamics Study on Coal Matrix Swelling Characteristics by CO2, N2, and CO2–N2 Mixture

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CO2 sequestration in coal seams is an economically viable option to reduce carbon emissions. Coalbed methane (CBM) is CH4 stored in the nanopores of the coal matrix. CO2 Enhanced CBM (CO2-ECBM) is considered prospective technology that can not only meet the increasing world energy resource demands but also ease greenhouse gas emissions by injecting CO2 into the coal seams. The injected CO2 is capable of promoting CH4 production. In the meantime, coal seams possess huge potentials for geological CO2 sequestration. However, the replacement process of CH4 in the coal matrix and the swelling/shrinkage of the coal matrix are poorly understood. Therefore, in this work, the molecular dynamics simulation study is presented considering the recovery of CH4 in the coal matrix and swelling of the coal matrix using CO2, N2, and CO2–N2 mixture, three different displacement schemes.

We quantify the amount by monitoring the density profiles. The results show that recovery of CH4 and swelling of the coal matrix are different in three displacement schemes. The use of CO2 injection obtained the highest recovery of CH4 inside the coal matrix. Meanwhile, coal matrix swelling is also quite severe. On the other hand, the use of CO2–N2 mixture injection yielded an increase of CH4 recovery as compared with the case of injecting pure N2. The coal matrix swelling is not severe. Also, there might be coal matrix shrinkage during the pure N2 displacement case. This work should shed light on the swelling of the coal matrix and recovery of CH4 during CO2, N2, and CO2–N2 mixture injection in coal seams.

