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Molecular concept of H_2O, CH4 and CO_2 adsorption on organic material

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Abstract

Unconventional gas, such as shale gas or coalbed methane offers an attractive low-carbon solution and furthermore provides possibilities for CO_2-storage and coevally for enhanced gas recovery. In order to better understand gas and water interaction with organic matter (coal) of different maturity we developed a molecular concept with experimental and literature support for sorption of these fluids on organic material over the entire range of thermal maturity. With increasing burial depth and temperature CO_2 and CH4 are the main volatiles released when organic material matures (cf. coalification). While most CO_2 is generally dissolved in formation water and transported away from the coal, most CH4 (coalbed methane, CBM) remains adsorbed to the coal pore structure and is produced as unconventional gas.

We present here the experimental basis and a conceptual model and to explain CO_2 and CH4 sorption in the presence of water on coal with varying coal maturity (from lignite to anthracite). Adsorption experiments have been performed on different maturity coals at various temperatures, pressures up to 20 MPa and under dry and moist conditions. With increasing coal maturity we find for both gases a linear sorption capacity trend for moisture-equilibrated and a more parabolic trend for dry coal samples. When investigating the difference in CH4 and CO_2 sorption capacity on coal of different maturity as a function of moisture content we infer that oxygen containing functional groups account for the selective sorption properties of gases and water to coals. Additionally restrictions in translational and vibrational movements of the sorbed gas molecules induced by adsorbed water molecules cause differences in the presence of water.