

## Diffusion of CO<sub>2</sub> in coal particles

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Sequestration of carbon dioxide in aquifers, hydrocarbon reservoirs or coal layers offer a promising alternative to reduce the amount of CO<sub>2</sub> released to the atmosphere. This contribution focuses on the sequestration in coal layers, in particular on diffusion. One advantage of sequestration in coal layers is that at the same time methane is displaced from the coal producing useful gas.

Injected gases mainly move through a vertical fracture system called cleats, shown in the figure. The cleats running from left to right are connected by “budd cleats” running from the bottom to the top. All pieces of coal bounded by the cleats contain a smaller fracture system until very small particulates with average diameters of 20 μm remain. These particles consist of a polymeric like structure that is originally derived from cellulose with the general formula C(H<sub>2</sub>O)<sub>n</sub>. During geologic times more or less of hydrogen and oxygen disappeared. As a result the particles contain hydrocarbon like parts and graphite like parts. The diffusion in the small particulates is extremely small and is therefore relevant for the efficiency of carbon dioxide sequestration in coal. The polymeric structure of coal is broken by the intruded CO<sub>2</sub> leading to swelling of the coal.

The swelling of coal matrix by the sorption of CO<sub>2</sub> is characterized by an anomalous diffusion process. Anomalous diffusion is indicative of the coupling of diffusional and relaxational mechanisms. Relaxation is related to the transition of coal from glassy to a rubbery state. It is claimed that for such anomalous diffusion the penetration rate in a slab is no longer proportional to the square root of time, but much faster. We explain a theory of the diffusion process of CO<sub>2</sub> in coal and its relation to matrix swelling based on extended non-equilibrium thermodynamics. The ensuing model equation is

$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial x} \left( D \phi \frac{\partial}{\partial x} \left( \ln \phi + \frac{\eta_l \Omega}{k_B T} \frac{\partial \phi}{\partial t} \right) \right).$$

where  $\phi$  is the volume fraction of CO<sub>2</sub> in the coal,  $D$  the diffusion coefficient,  $\eta_l$  the elongational viscosity coefficient,  $\Omega$  the molecular volume and  $k_B$  the Boltzmann constant. Some aspects of anomalous diffusion based on this equation and its boundary conditions will be discussed.