

## Dynamics of water in compacted clay systems

F. Jurányi (1, 2), F. González (1), L. Van Loon (1), T. Gimmi (1, 3), T. Seydel (4)

- (1) Paul Scherrer Institute, 5232 Villigen PSI, Switzerland
- (2) University of Saarland, 66123 Saarbrücken, Germany
- (3) University of Bern, 3012 Bern, Switzerland
- (4) Institut Laue-Langevin, 38042 Grenoble, France

Compacted clays and argillaceous rocks are widely used as barriers around disposal sites of hazardous wastes because of their well-suited physico-chemical and hydro-logical properties. The pores in compacted clays are so narrow that only a few water layers can be build up. Water in close vicinity to the surface of clay has properties different from bulk liquid water [1]. This might have several implications for the thermodynamics of water, solutes and for the diffusive transport of pollutants in such barriers. In order to predict the rates of diffusive transport and design effective waste disposals, it is essential to understand the microscopic diffusion process of confined water.

Four clays with systematic structural differences have been investigated:

Na-montmorillonite, Na-illite, Pyrophyllite (all with a TOT layer structure (T: Si tetrahedral, O: Al octahedral [2]) and Kaolinite (with a TO structure). In Na-montmorillonite water is located in between clay particles and in the interlayer space. In the others water is placed only in between the particles. The TOT layers of Na-illite are more tightly linked by potassium cations. Pyrophyllite and Kaolinite have no interlayer structure due to their charge neutrality within the sheets.

Diffusion of water in these clays is being studied at two spatial scales (macro- and micro-scale) in order to get a complete description of the diffusive motions. The macroscopic diffusion is strongly affected by the geometry of the pore space, the microscopic diffusion not. Therefore, a comparison of the two scales can be done by the activation energy. The microscopic diffusion was studied with quasielastic neutron

scattering performed at the time-of-flight spectrometer FOCUS (SINQ, Paul Scherrer Institut). Using the jump diffusion model [3], a large dependency of the diffusion coefficient and residence time on clay structure was found.

The activation energy seems to differ from that of bulk water only in clays with interlayer space. Measurement with higher resolution was performed at the backscattering spectrometer IN10 (ILL). The intensity of the elastically scattered neutrons as a function of temperatures below  $0^{\circ}$ C (i.e. the freezing behaviour) is strongly affected by the clay structure.

## **References:**

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[2] K.B.Krauskopf. Introduction to Geochemistry. Mc Graw-Hill.1979

[3] M. Bèe: Quasielastic Neutron Scattering. Principles and Applications in Solid State Chemistry, Biology and Materials Science. Adam Hilger, Bristol and Philadelphia. 1988.