

Modelling of multicomponent ion transport in compacted bentonite

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Molecular diffusion will be the dominant transport mechanism in a compacted bentonite barrier of a nuclear waste repository due to its high content of montmorillonite and the control that this clay mineral exerts on the porewater distribution in bentonite. A multicomponent advective-diffusive transport experiment was performed for 304 days at laboratory scale with a cylindrical column of compacted MX-80 saturated bentonite. The column was isolated and confined under water pressure, and an artificial saline solution was infiltrated from one end of the column. The outflow solution was collected in syringes at the other end. The geochemical reactive transport code PHREEQC [1] was used, implementing a multi-porous system and anion exclusion induced by swelling of the expandable clay fraction in compacted bentonite and by the formation of electrical double layers (DDL) on charged surfaces [2], in addition to mineral equilibrium with accessory minerals, ion exchange and multicomponent ionic diffusion. The DDL is optimized by the Cl⁻ evolution to occupy ~85 % of the pore volume, assuming that this anion can only migrate in the “free pore water”. D₂O breakthrough was also used to constrain transport parameters.

The model shows good agreement with the experimental results and demonstrates the important role of the DDL and interlayer pore waters controlling the ionic mobility. The model can explain the slow release of SO₄⁻² out of bentonite and accumulation of Ca⁺² in bentonite by gypsum and calcite dissolution and predicts ion exchange of Ca⁺² for Na⁺ at the interlayer of montmorillonite. The sensitivity of the parameters to assumptions regarding porosities and anion-exclusion are evaluated.

[1] Parkhurst & Appelo (1999) *USGS Water Resources Investigations Report 99-4259*. [2] Appelo & Wersin (2007) *Env. Sci. Tech.* **41**, 5002-5007.

Cycles and origin of ultrafine and black carbon particles in Huelva city (SW Spain)

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The physical characterization of metrics representative of the particle concentration, complementary to PM₁₀ and PM_{2.5}, has become a matter of high interest within the context of air quality and human exposure assessment. We present a study on ultrafine particles (measured as the number concentration of particles ≥ 2.5 nm, N_{2.5}) and black carbon particles (BC less than $\leq 10\mu\text{m}$) performed in Huelva city (SW Spain).

It was found that road traffic was the most important source contributing to the levels and variability of BC. Because of the vehicle exhaust emissions, BC exhibited daily cycles similar to those of NO_x. The highest BC concentrations were recorded during the morning rush hours of the working days, whereas the daily evolution of BC was significantly different during weekends. Concentrations of N_{2.5} were high, and correlated with those of BC, during the morning rush hours owing to the vehicle exhaust emissions.

During the noon – afternoon period, when BC concentrations were low, high N_{2.5} levels were still recorded. The N_{2.5}/BC ratio exhibited a daily evolution highly correlated to that of the solar radiation intensity. These high N_{2.5} levels were correlated with the arrival to the measurement site of SO₂ plumes from the industrial area located at the south of the city.

It is concluded that, in addition to vehicle exhausts, industrial emissions of gaseous precursors, significantly contribute to the ultrafine particle concentration.