Coupling the gas phase to reactive transport to model the oxic transient stage in radioactive waste disposals

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The coupling of the gas phase to reactive transport is a key issue for modeling the subsurface exploitation. Two studies were recently performed with the HYTEC code. A multiphase multicomponent benchmark was proposed on the long-term evolution of a CH_4 gas reservoir with significant contents in sour gases CO_2 and H_2S [1]. The second study, presented here, dealt with the oxic transient stage during the exploitation of geological radioactive waste disposals [2].

The spatial extent and duration of the oxic transient stage are important factors for performance assessments of disposal in argillaceous formations, e.g. for metallic components that may undergo high corrosion rates under such conditions. Studies carried out in the argillite formation of Tournemire (France) showed that oxic conditions could last several years in boreholes [e.g. 3], which were sealed but presented axially disturbed zones due to drilling.

The balance between i) the kinetics of oxidative dissolution of pyrite from the host-rock, ii) the kinetics of carbon steel corrosion and iii) the diffusion of oxygen gas in the water unsaturated rock along the cell is analyzed in a disposal cell at atmospheric pressure and 20 °C during 100 years. In a closed system, modeling leads to a complete and fast consumption of oxygen. Under open ventilated conditions, a redox contrast may occur between reducing conditions at the back of the disposal cell (with anoxic corrosion of steel and hydrogen production) and oxidizing conditions at the front (with oxic corrosion of steel). The extent of the oxidizing/reducing front in the disposal cell is strongly dependent on the gas diffusion coefficient in partially saturated zones.

[1] Sin *et al.* (2015) *MAMERN VI*, June 1-5, Pau (France), 18p.
[2] De Windt *et al.* (2014) *Appl. Geochem.* 41, 115-127. [3] Gaudin *et al.* (2013) *Appl. Clay Sc.* 83-84, 457-468.