

## **THEME 4:**

### **The Earth's Surface**

#### **Session 4:3**

#### **Rates and mechanisms of biogeochemical processes**

CONVENED BY:

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Biological activity plays a major role in determining the chemical structure and evolution of the Earth's surface, including marine and coastal basins, lakes, estuaries, soils, sediments and aquifers. These environments are sites of extensive transformation and cycling of nutrients and metals. They also offer a variety of geochemical habitats in which organisms and abiotic reactions compete for available chemical substrates. Recent decades have witnessed rapid developments in understanding the complex reaction pathways in biogeochemical systems. The goal of this session is to highlight the emergence of novel approaches and theoretical models, which allow researchers to measure, rationalise and predict in situ rates of biogeochemical transformation in natural and engineered systems. We invite field-oriented, laboratory-based and modelling contributions that offer quantitative insight into the dynamic functioning of biogeochemical systems. Particularly welcome are contributions that: 1) combine observations of reaction pathways and kinetics with reactive transport modelling in order to derive in situ rate distributions of biologically-driven processes, and 2) integrate a characterization of the biogeochemical processes.

#### **4.3.11**

#### **Modeling biogeochemical oxygen reduction in fractured granites**

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Several countries around the world are considering deep repositories in fractured granitic formations for the final disposal of high-level radioactive waste. Evaluating the long term safety of such repositories requires sound conceptual and numerical models which are being developed from data and knowledge gained from in situ experiments carried out at deep underground laboratories such as that of Äspö in Sweden. One of the key aspects for performance assessment concerns to the behaviour of dissolved oxygen because it will affect to the corrosion of canisters. Moreover, several long-lived radionuclides are much more soluble and mobile under oxidizing conditions.

The REX project (Redox Experiment in Detailed Scale) was carried out during the years 1998-2001 at the Äspö Hard Rock Laboratory. The main objective of the REX project was to investigate dissolved oxygen depletion by creating controlled oxidising perturbations in a deep rock environment (380 m depth), which is representative of deep repository conditions. Field experiments were based on the injection and monitoring of non-reactive tracers and dissolved oxygen. Oxygen pulses were injected into a wide borehole reaching a fracture surface which was hydraulically isolated by packing a borehole section. In general, observed oxygen consumption took place in less than a week.

Coupled biogeochemical reactive transport models have been developed to simulate these in situ experiments. Numerical models account for molecular diffusion through the rock, abiotic hydrogeochemical reactions and microbial processes. Numerical models have been used to reproduce measured rates of oxygen consumption, taking into account the structure of microbial populations found in Äspö groundwaters. Numerical models also incorporate information and parameters obtained through laboratory experiments. It has been evaluated that aerobic respiration of organic matter and microbially-driven methane oxidation are the main processes responsible of oxygen reduction. On the other hand, pure abiotic consumption of dissolved oxygen has been computed to occur in a period of about 1,000 years. Then, it is concluded that autochthonous biogeochemical mechanisms accelerate drastically the kinetics of oxygen uptake, which can be highly relevant to evaluate the performance of a deep geological repository.