Prediction of the key physico-chemical parameters of geological barriers through detailed mineralogical analysis: case study of the Boom Clay (Belgium)

Lander Frederickx [1,2], Miroslav Honty[1], Norbert Maes[1] & Christophe Bruggeman[1]
[1] Belgian Nuclear Research Centre, SCK•CEN, Mol, Belgium
[2] Department of Earth and Environmental Sciences, KU Leuven, Belgium
E-mail: mhonty@sckcen.be

Context & Objectives

Clay host rocks play a central role in the geological disposal concepts of several countries, as they will be responsible for the long-term retention of radionuclides. An in-depth characterization of the host rock is necessary to gauge the sorption and retention capacities of the formation as a whole. Key characteristics include the grain size, mineralogy, cation exchange capacity (CEC), specific surface area (SSA), etc.

It is unfeasible to measure all these properties in detail on a formation scale, so we demonstrate a cost-effective way to acquire as much information as possible with a relatively small characterization campaign. The properties mentioned above are measured in a small sample set representative of the host formation. The acquired data is used as a training set for a statistical model, in which all properties are predicted by using the grain size distribution. This translates into a significant reduction of the analyses required to characterize a host formation in detail.

Training data

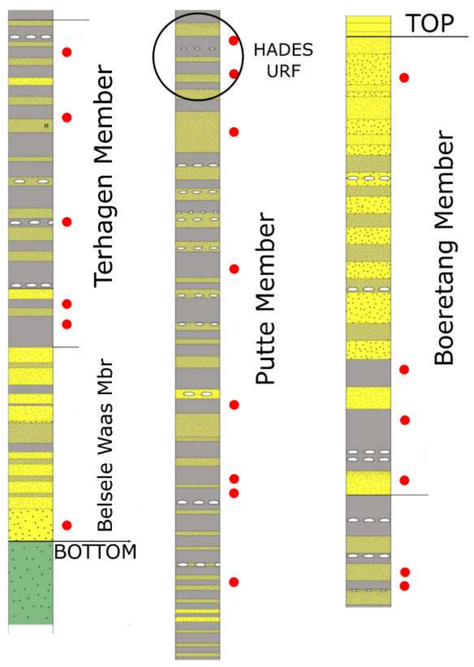

Figure 1: Stratigraphic positions of the training data in the Boom Clay.

Samples

- Boom Clay formation
- ON-Mol-1 borehole
- 20 samples from all stratigraphic members

Methods

- **Mineralogy** X-Ray Diffraction
- **Grain Size** SediGraph
- **CEC** Exchange of Cu-trien
- **SSA** N_2 physisorption (BET)

Grain Size Data

- Boom Clay samples
- ON-Mol-1 borehole
- 213 SediGraph measurements from present and past studies

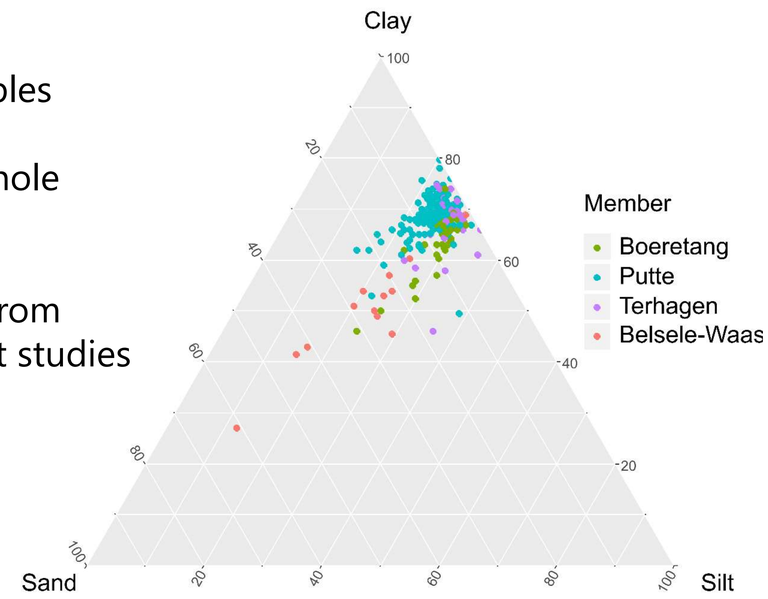

Figure 2: Ternary diagram of all 213 grain size measurements.

Predicting mineralogy with grain size data

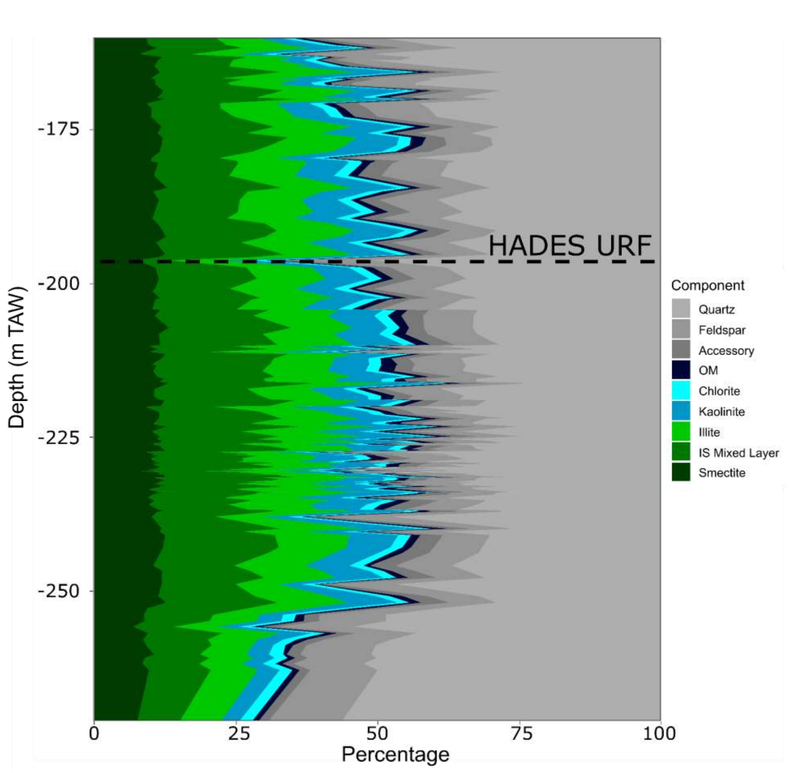

Figure 3: Predicted mineral compositions

Centered log ratio transformation (CLR) of data to a compositional space

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Partial least squares (PLS) regression to individually predict each mineralogical component

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Inverse CLR transformation to normal space

Predicting CEC and SSA with grain size data

Separate PLS regressions to predict CEC and SSA

Both CEC and SSA show similar trends, which coincide with the predicted trend in the mineralogy

The same approach can be applied for other parameters

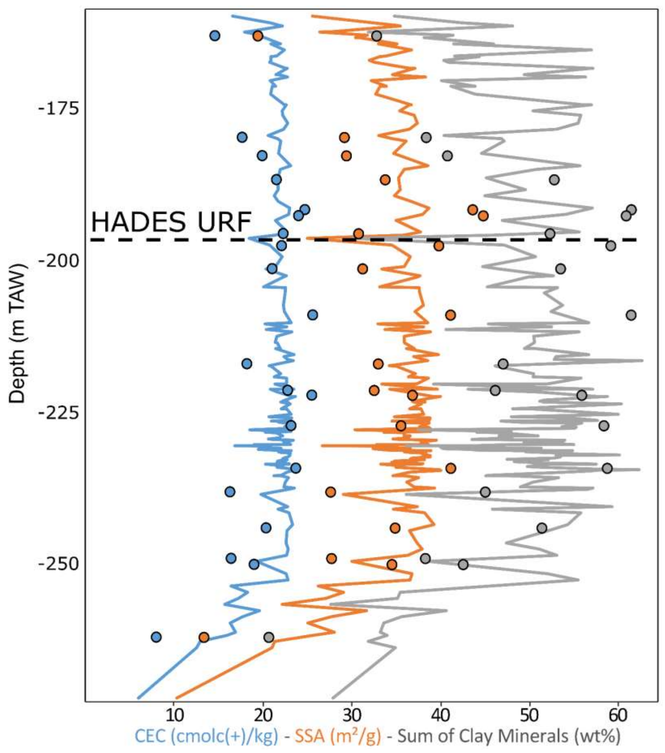

Figure 4: Predicted CEC and SSA values. Circles indicate the training data.

Conclusion & Perspectives

- A relatively small training set, characterized in detail, combined with a large data set of grain size measurements, proved sufficient to predict key physico-chemical parameters and mineralogical components of the Boom Clay formation.
- This approach can be adapted to other (clay) formations and clay properties.
- In order to further reduce analysis requirements, we are looking into relating the properties of the clay host rock to well logging measurements (i.e. NMR, μ-resistivity). If successful, a full prediction of these properties can be made for the entire logged profile.

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