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Towards Digital Twins: Uncertainty and Sensitivity Analysis for Safety-Case Modelling

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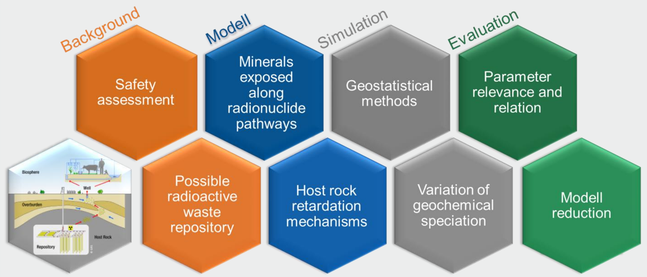
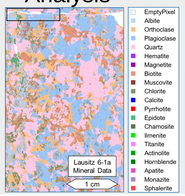
Motivation

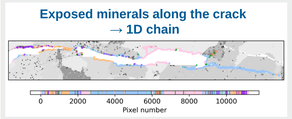
- Deep geological repositories require **robust, science-based safety concepts** for long-term radioactive waste storage.
- Digital twins (DT) can **represent, visualize, and test complex geosystem** behavior in data-rich safety cases.
- To ensure consistent DTs, the **relevant parameters, processes, and scales** must be identified.
- **Uncertainty and sensitivity analyses** provide the basis for **compact, interpretable, and reliable** DTs.
- Case study: simulation of **radionuclide (RN) retention** in a **crystalline** host rock.

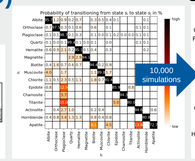


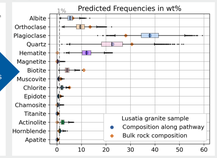
1 Geostatistical Simulation

- **Crystalline rock** (granite)
- Thin sections analyzed by Mineral Liberation Analysis
- Simulation approach:
  - **Markov Chain (1D)**
  - Truncated **multi-Gaussian Random Fields (2D)**
- Many realizations → **Variability of mineral composition**
- Exposed mineralogy along pathways



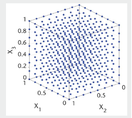






2 Model Parameterization

- Input sample generation:
  - **Quasi-Monte Carlo**
  - **Stick-Breaking** (compositional data)



Mineral composition + uncertainty
Based on the analysis of five thin sections

Parameter	Lower limit / wt%	Upper limit / wt%	SCM data
Albite	0,0	84.8	+Plagioclase
Orthoclase	0.2	82.2	
Quartz	0.0	53.7	
Hematite	0.0	19.3	Goethite
Biotite	0.0	34.0	Phlogopite
Muscovite	0.0	10.8	Illite
Chlorite	0.0	12.8	Clinochlore
Epidote + others (<1wt%)	0.0	9,3	*Residuals*

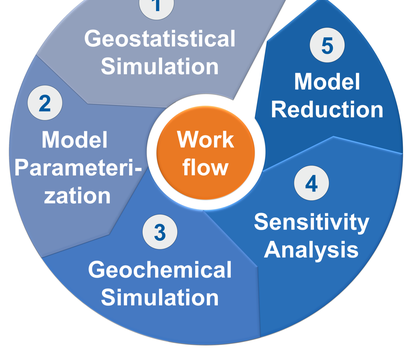
Good data (surface complexation models – SCM) available

No SCM data available → replaced by a chemical analog

Minerals very rarely in the Lusatian granites (< 1 wt%) + no SCM data is available → considered as "Residuals"

Pore/fracture water composition + uncertainty

Parameter	Lower limit	Upper limit	Unit	Parameter	mol/l
UO_2^{2+}	$4.0 \cdot 10^{-8}$	$5.0 \cdot 10^{-6}$	mol/l	SO_4^{2-}	$8.5 \cdot 10^{-4}$
pH	5.0	9.0		Na^+	$2.0 \cdot 10^{-3}$
E_h	−300	100	mV	NO_3^-	$5.2 \cdot 10^{-4}$
SLR	0.5	3.5	g/l	Mg^{2+}	$3.2 \cdot 10^{-4}$
Ca^{2+}	$0.1 \cdot 10^{-4}$	$16.0 \cdot 10^{-4}$	mol/l	Cl^-	$2.0 \cdot 10^{-3}$
HCO_3^-	$4.5 \cdot 10^{-4}$	$5.5 \cdot 10^{-4}$	mol/l	K^+	$2.1 \cdot 10^{-4}$



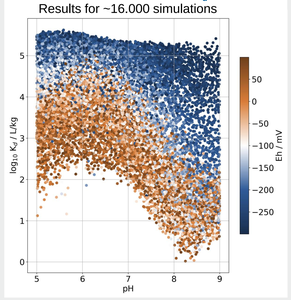
3 Geochemical Simulation

- Tool: The Geochemist's Workbench
- **RN retention**:
  - Sorption (surface complexation)
  - Aqueous speciation
  - Precipitation/ dissolution

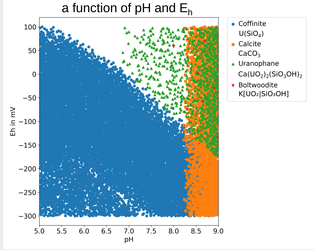
Distribution Coefficient

$$K_d = \frac{[RN]_{solid/immobilised}}{[RN]_{dissolved/mobile}}$$

Distribution Coefficient K_d
Results for ~16.000 simulations



Minerals in system
Precipitated minerals as a function of pH and E_h

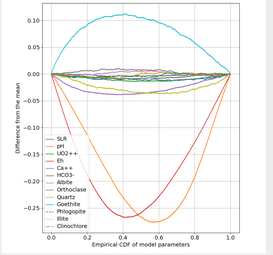


4 Sensitivity Analysis

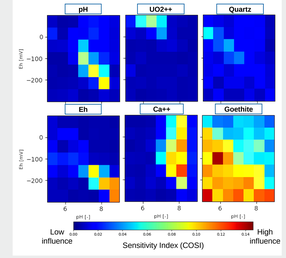
- **Variance-based** sensitivity analysis methods
- 1st order: **Influence** of parameters on K_d values
- 2nd order: Pairwise parameter **interactions**

SA Toolbox
User manual, theory manual & software releases

CUSUNORO plot
Cumulative Sum of Normalized Reordered Output (CUSUNORO)
Large amplitude → Parameter variation leads to strong changes in K_d



Checkerboard analysis
Cosine Sensitivity Index (COSI) as a function of pH and Eh



Take Home Message

Our workflow allows to
- provide **uncertainties in mineral composition**,
- determine **RN retention properties**,
- identify **relevant parameters** and their correlation.

Its application can be extended to
- other **host rocks (clay, salt)** and
- any number of radionuclides.

The SA provides **guidance for digital twin design**:
- High-relevance parameters: represented as spatially variable parameters with high resolution and precision.
- Low-relevance parameters: treated as constants globally or within subsections.

5 Model Reduction

- Based on the sensitivity analysis (SA) most sensitive parameters are identified:
  pH, E_h, Uranium, Calcium, Quartz, Goethite
- Behavior of a **parameter's impact** across its range of values can be described **quantitatively**.
- Model reduction becomes possible:
  - Set parameters with low sensitivity to **constant**
  - **Restrict** value ranges
  - **Merge** parameters

References

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