PAUL SCHERRER INSTITUT

PSI

Wilfried Pfingsten, Luca Podofillini :: NES/LES,LEA :: Paul Scherrer Institut

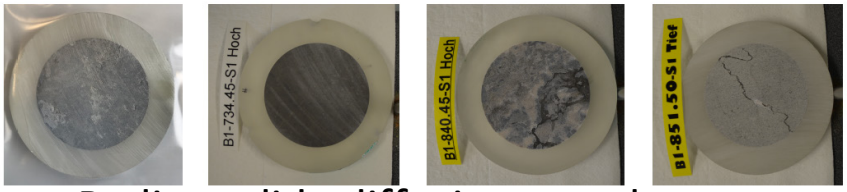
Semester-/Master Thesis at LES,LEA

Nuclear Master Info at PSI, 17th May 2021

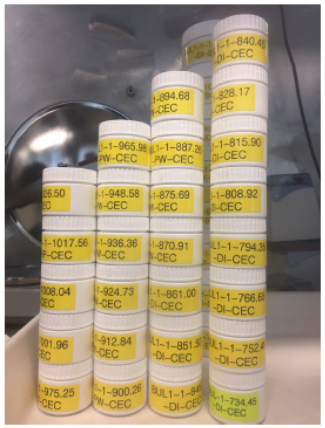
Laboratory for Waste Management (LES)

LES is the **Swiss competence center** for **geochemistry** and **multiscale radionuclide** and **mass transport** in **argillaceous rocks** and **cement** and their **application to deep geological systems** and **Swiss radioactive waste repositories**.

At the moment, we are strongly involved in sorption measurements and through diffusion experiments with samples from deep boreholes near potential repository sites in northern Switzerland (Sectoral Plan, phase 3).



Radionuclide diffusion samples



26 TBO samples for CEC

https://www.psi.ch/de/les

Expertise of LES

Basics of repository chemistry:

thermodynamic databases, solubility of radionuclides,
geochemical equilibrium codes

Chemistry at the solid /liquid interface:

laboratory sorption experiments and mechanistic sorption models,
molecular modelling, microscopic sample characterisation

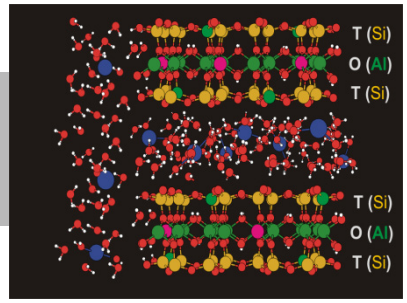
Mass transport mechanisms:

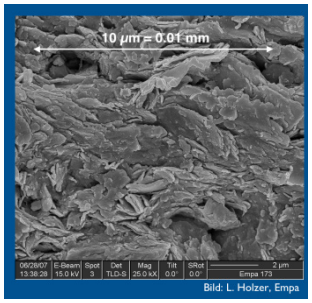
diffusion and precipitation/dissolution experiments and multi-scale modelling,
coupling of chemistry and transport, code development
apply machine learning for reactive transport processes,
parameter uncertainty propagation for radionuclide migration
digital twin development

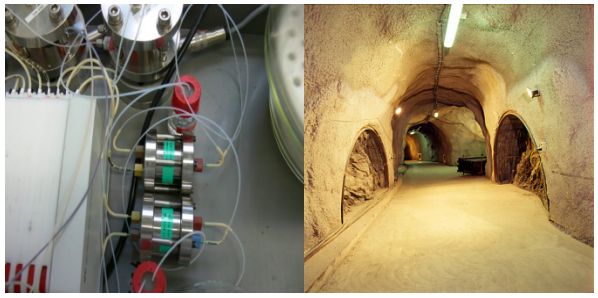
Participation in performance assessments:

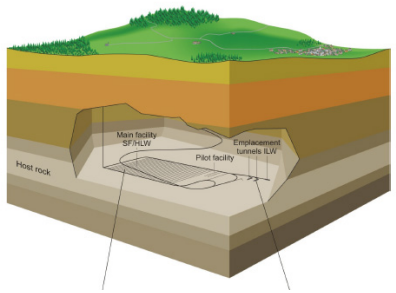
databases for solubility, sorption, diffusion coefficients of radionuclides
state-of-the art review reports

LES Research - Processes and Scales





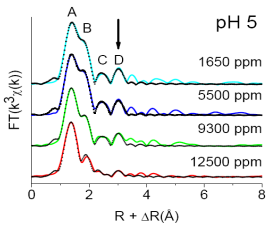


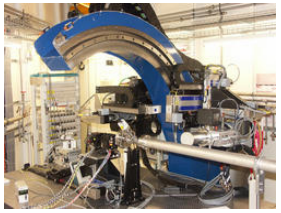


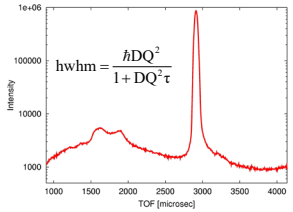
ns μs ms s days y 10^3y *time*

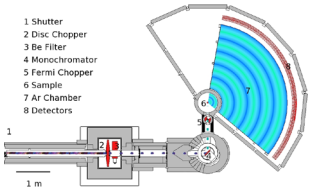
nm μm mm m km *distance*

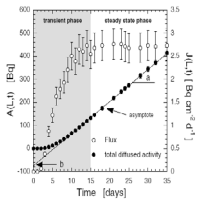
Moleculare Diffusion/Sorption	Reaction Kinetics Dissolution/Precipitation	Modelling of Lab and Field Experiments	Modelling of Repository Evolution and RN Transport

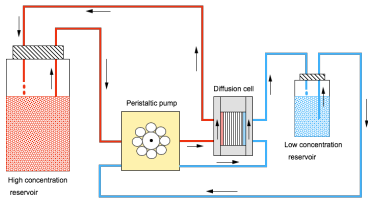


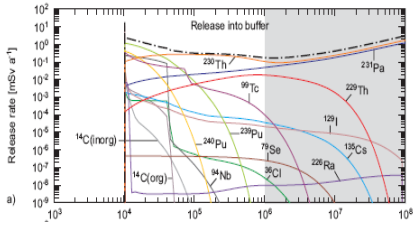


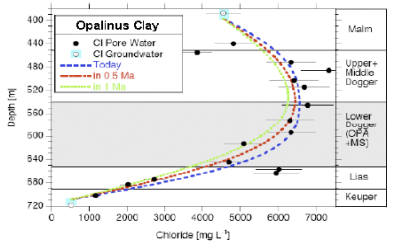








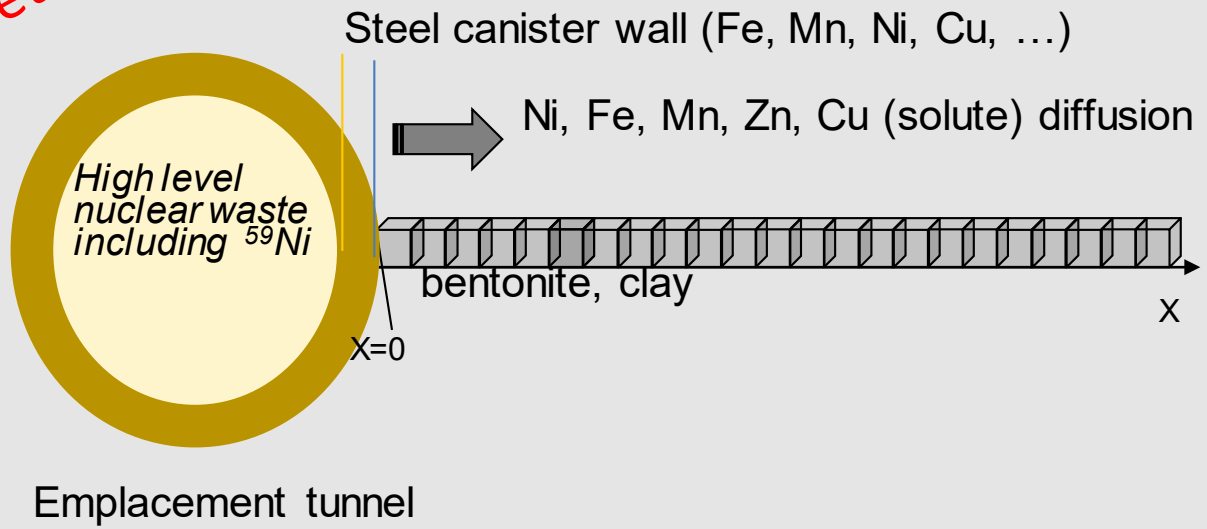




^{59}Ni diffusion into bentonite – sorption competition with other bi-valent cations

Ni(II) release from the canister wall into the bentonite in parallel with leaching of other bivalent elements originating from steel canister corrosion or waste.

Project: Model Setup



Use data from deep bore holes for modelling of Ni migration

Sorption model parameter - uncertainty

Selectivity coefficients, K_c, for Ni and Zn and other bivalent cations used in the calculations.

Cation exchange reactions on planar sites Na-mont (montmorillonite)	$LogK_c$
2 Na-mont + Ni^{2+} ⇔ Ni-mont + $2Na^+$	0.5 Bradbury, 2011 #1456} 3.1 (Bradbury and Baeyens, 1997)
2 Na-mont + Fe^{2+} ⇔ Fe-mont + $2Na^+$	"same as for Ni"
2 Na-mont + Mn^{2+} ⇔ Mn-mont + $2Na^+$	"same as for Ni"
2 Na-mont + Zn^{2+} ⇔ Zn-mont + $2Na^+$	3.9 Na-Milos &STX-1 (Dähn et al., 2011) 3.9 (Bradbury and Baeyens, 1997)
2 Na-mont + Cu^{2+} ⇔ Cu-mont + $2Na^+$	"same as for Ni"

Sorption model parameters in red: values with uncertainty or not known

LES/LEA proposal for Semester + Master projects:

Numerical simulations

Sorption competition parameter uncertainty for reactive transport modelling of Ni diffusion through bentonite

For a **semester project**, the student will get familiar with the codes used for coupling chemistry to transport processes by doing a simple, already known example of modelling reactive transport with sorption and learn about procedures to investigate parameter uncertainty with respect to reactive transport modelling.

For a **master thesis**, model calculations will be performed that investigate parameter uncertainty (e.g. sorption model parameters) and its influence on radionuclide (e.g. ^{59}Ni) diffusion and calculated breakthrough curves in bentonite.

Prerequisite: Some basic knowledge in chemical thermodynamics and radionuclide migration and sorption processes and statistical methods.

Contact: wilfried.pfingsten@psi.ch

Last thesis:

Applied Geochemistry
Volume 117, June 2020, 104607

Uncertainty and sensitivity analysis of the chemistry of cesium sorption in deep geological repositories

Ali Ayoub [a], Wilfried Pfingsten [b], Luca Podofillini [c], Giovanni Sansavini [a]

Show more

https://doi.org/10.1016/j.apgeochem.2020.104607

Get rights and content

Highlights

- Methodology to study uncertainties of sorption parameters of Cesium in clay.
- Identifies most important model parameters affecting uncertainty in Cesium sorption.
- New Cesium isotherms and Kd band based on detailed sorption chemistry uncertainties.
- Help designing laboratory experiments and inform repository performance assessment.
- Applicable to any complex reactive transport problem and any radionuclide.

Wir schaffen Wissen – heute für morgen

Mein Dank geht an

All of you for listening