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NUMERICAL MODELLING OF BENTONITE EROSION DUE TO SEDIMENTATION IN SLOPING FRACTURES

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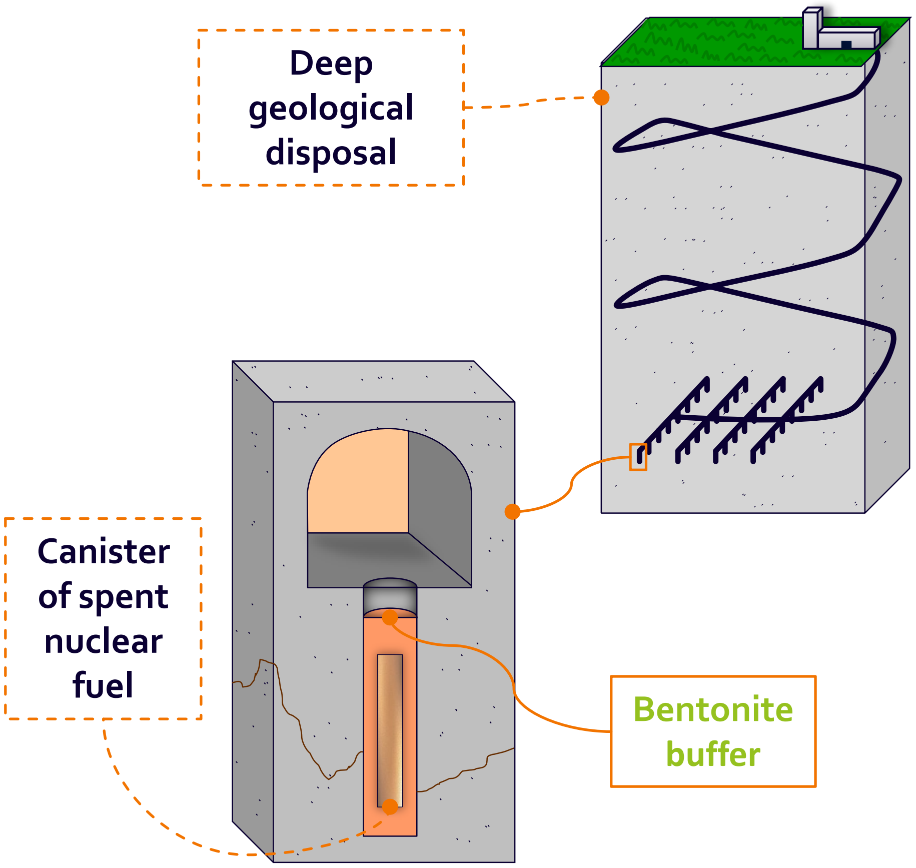
Introduction

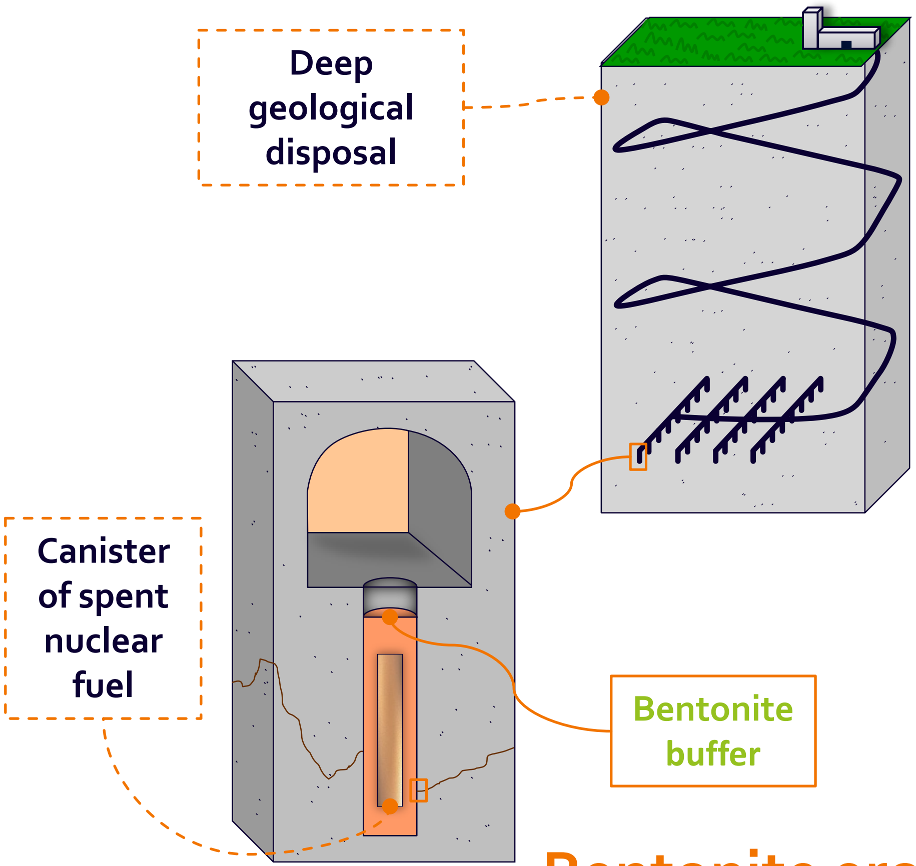


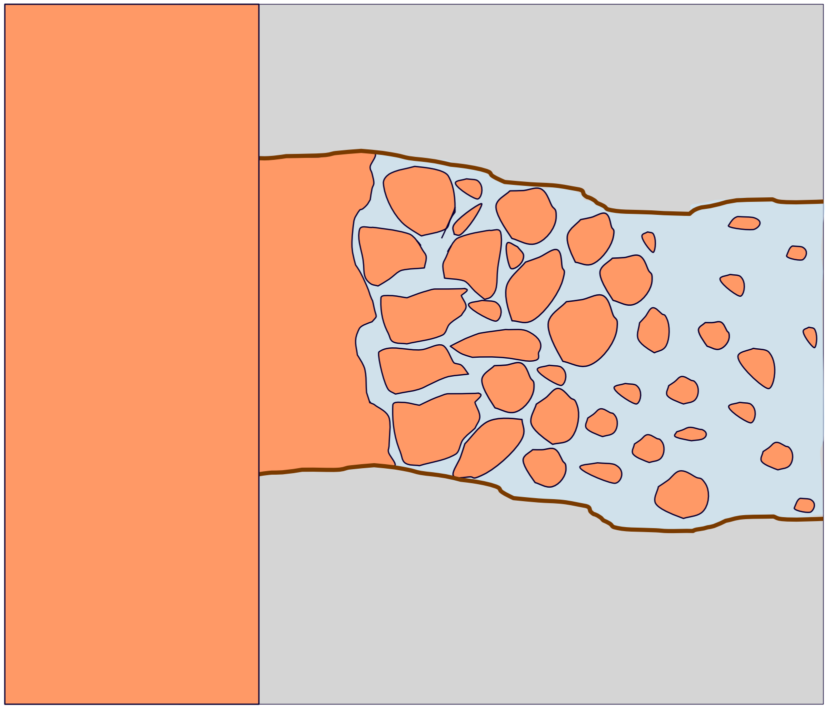
Bentonites are an active clay that presents several properties such as:

- *high swelling potential*
- *high retention capacity*
- *low hydraulic conductivity*

Due to its properties, **bentonite** has been selected as the **engineering barrier** between the encapsulated radioactive waste and the bedrock (**buffer material** and **tunnel backfill**).

Introduction





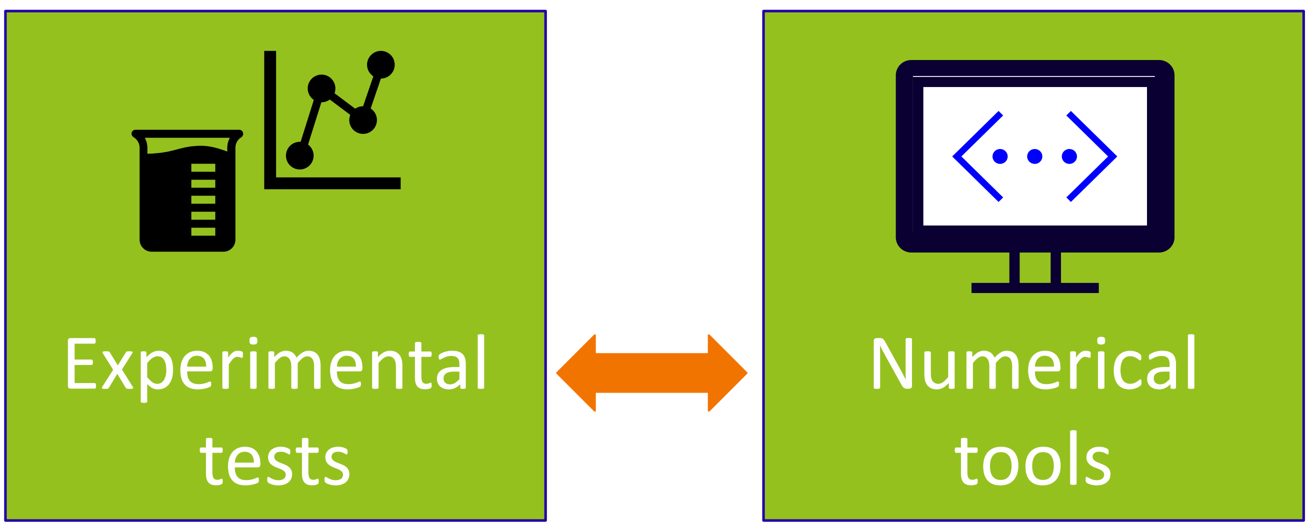
Bentonite erosion mechanisms in fractures

- Mechanical erosion due to shear by seeping water
- Sedimentation due to flocculation (chemical erosion)
- Sedimentation due to gravity in sloping fractures

Introduction

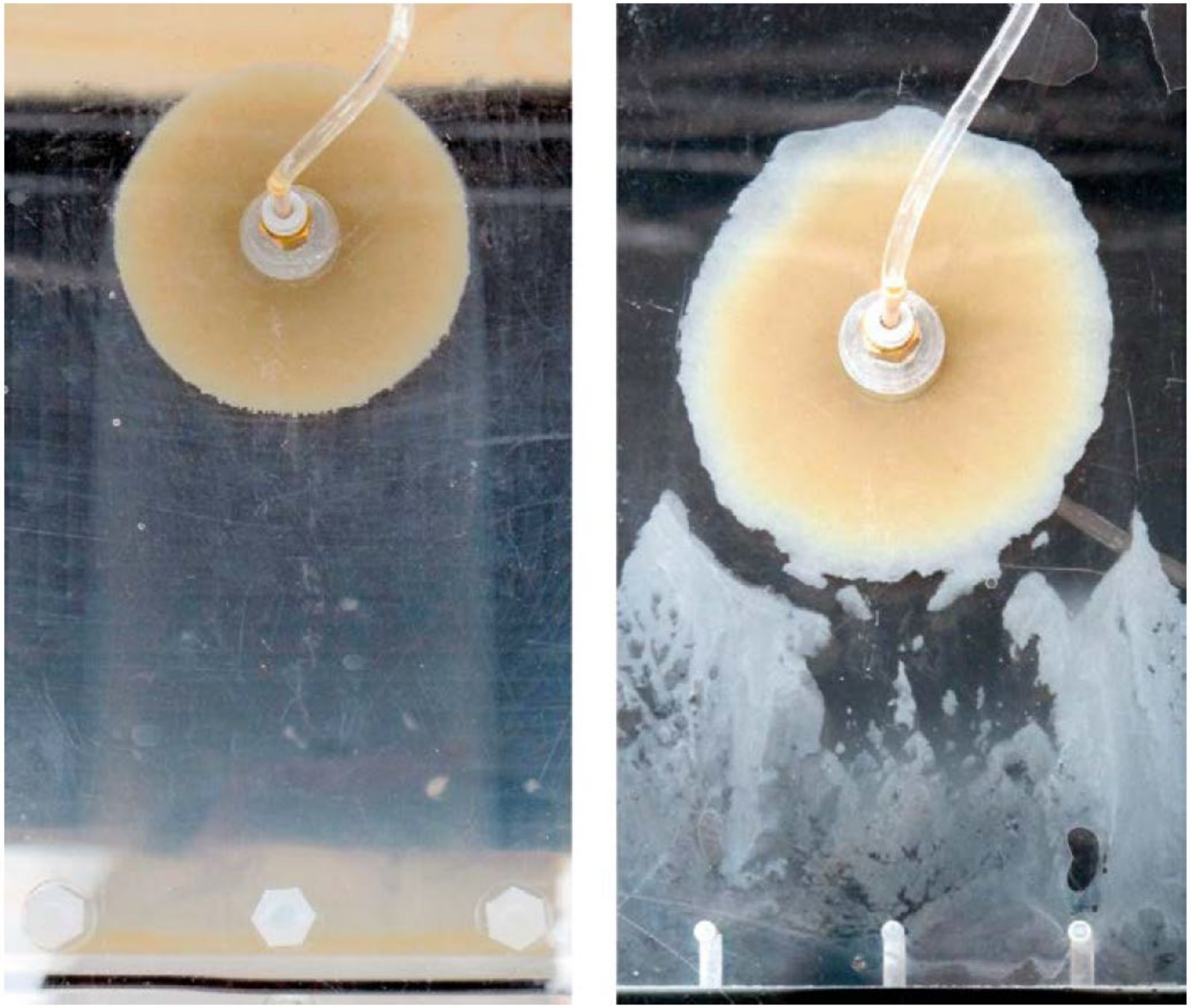
Objective

The study of **bentonite erosion mechanisms in fractures** is a problem of maximum interest in understand their impact on the *long-term performance* of the bentonite buffer.



Introduction

Experimental tests of bentonite pellet in narrow fractures



Images of extrusion and mass loss of sodium montmorillonite in 45° sloped fractures with 1 mm apertures, left and 0.1 mm. Simulated Grimsel water, GGWS, with Na^{+} 0.68 and Ca^{2+} 0.14 mM (Schatz and Akhanoba 2016).

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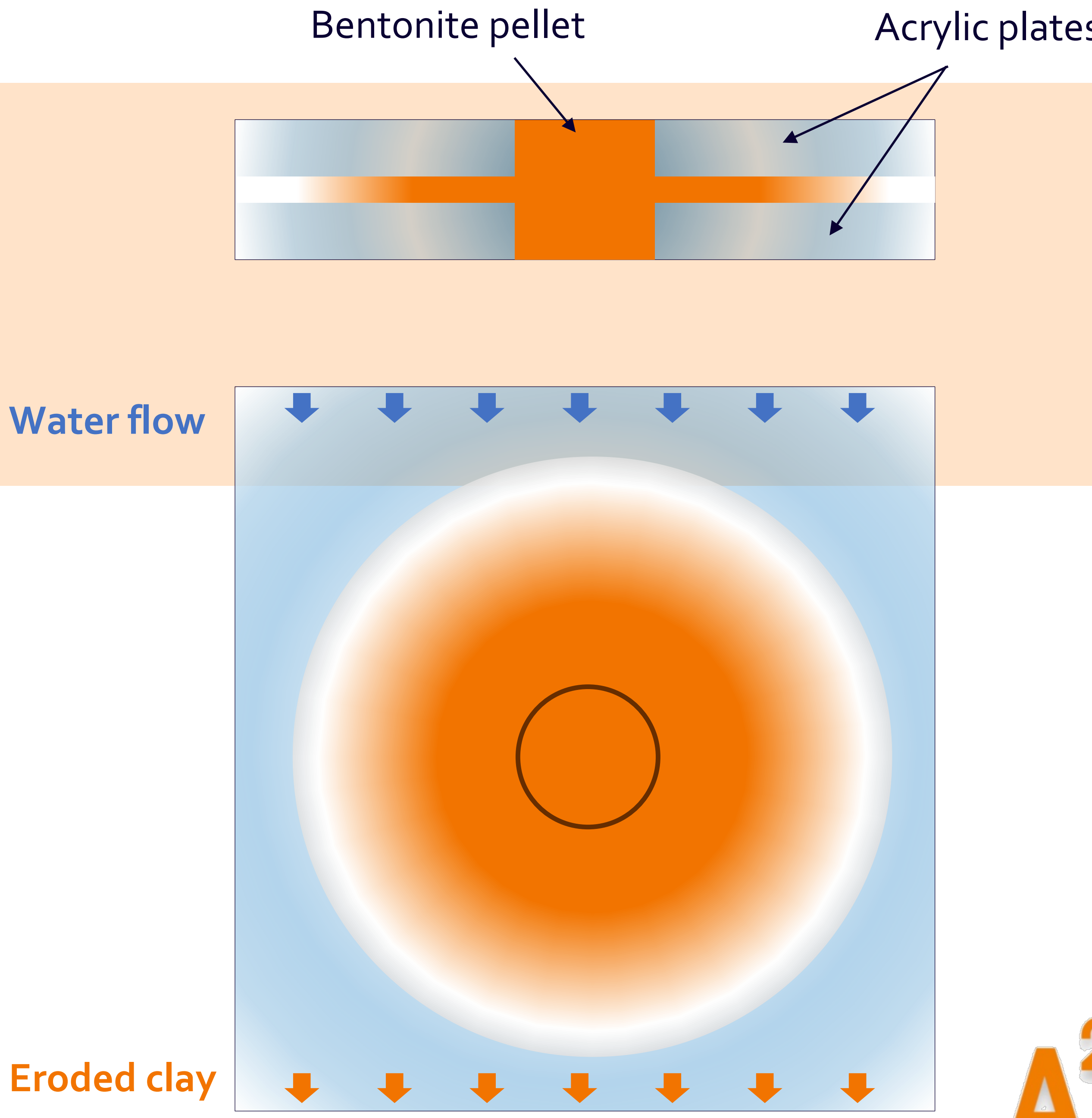


Conceptual model

Model for bentonite expansion and erosion by Neretnieks and co-workers [1] accounted for:

- **Expansion of the smectite in the fracture**:

  balance between

  - the *repulsive* Diffusive Doble Layer forces
  - the *attractive* van der Waals forces

- **Mechanical erosion due to shear by seeping water in the fracture**

[1] (Liu et al. 2009, Moreno et al. 2010 and Neretnieks et al. 2009)

Conceptual model

Based on the bentonite expansion and erosion model by Neretnieks and co-workers [1], **Amphos 21** has developed a model with the following features:

Wall friction model

Shear resistance against expansion exerted by the accumulation of segregated flocs at the rim (interface bentonite-water)

Sedimentation model

Gravity effect

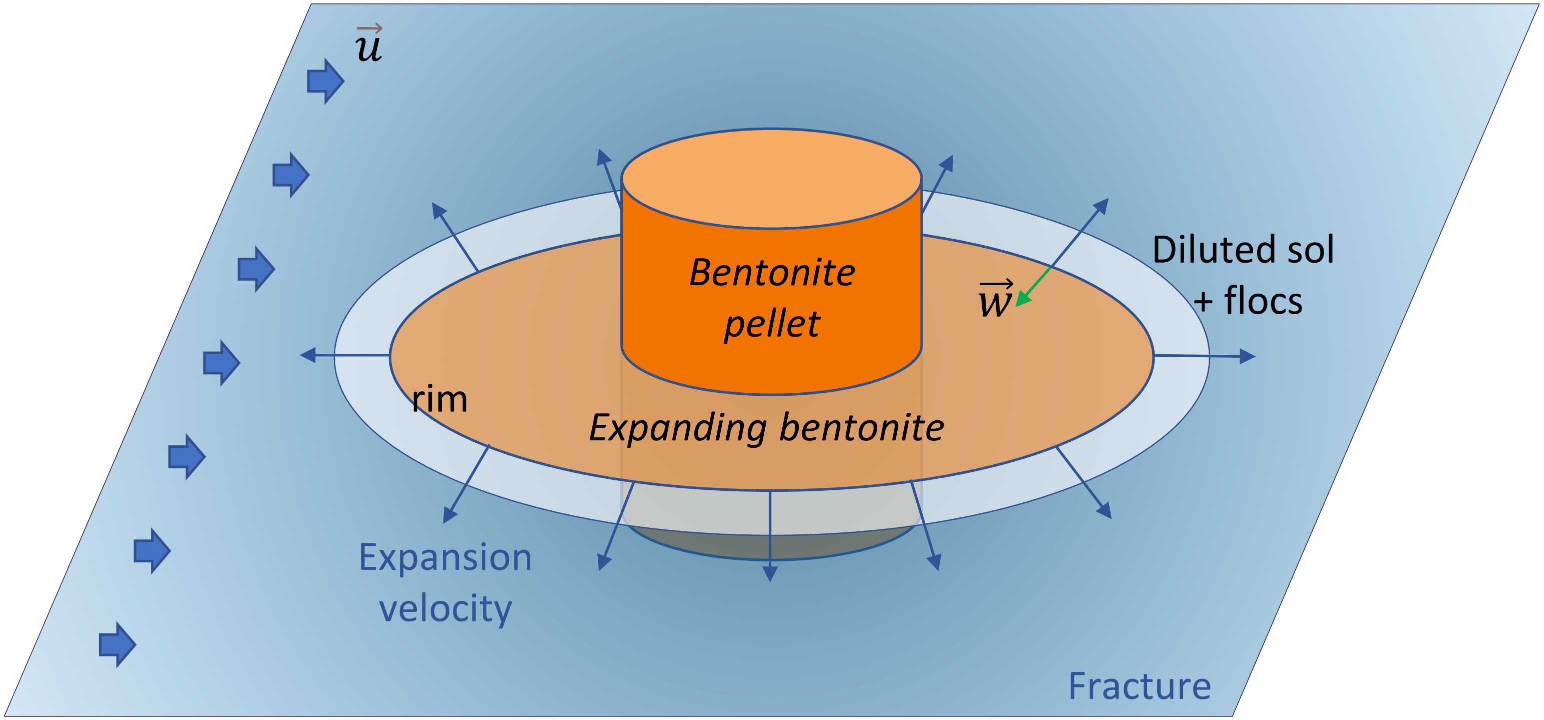
*The **sloped fractures** intersecting bentonite have a higher **erosion rate** than horizontal ones.*

[1] (Liu et al. 2009, Moreno et al. 2010 and Neretnieks et al. 2009)

Conceptual model

Bentonite volume fraction | Wall friction | Expansion | Flow

$$\partial_t \varphi = -\nabla \cdot (\vec{w}\varphi) + \nabla \cdot \left(\frac{\chi}{f} \nabla \varphi\right) - \vec{u} \cdot \nabla \varphi$$



Conceptual model

Wall friction model

Shear velocity

$$|\vec{w}| = \frac{\tau_1 \delta}{4\,\eta_{\mathrm{eff}}}\, f(r, \delta, [\mathrm{Na}^+])$$

- The wall friction term has been correlated with fracture aperture according to the Herschel-Bulkley flow model (for viscous shear stresses)
- Rim thickness has been correlated with sodium concentration at the rim (c_{rim})

Conceptual model

Sedimentation model

Settling velocity $$u_p = \frac{g(\rho - \rho_w) d_p^2}{18 \eta_w}$$

$$d_p = d_{p0} \left(\frac{\delta}{\delta_0} \right)^{\alpha}$$

$$\kappa = \frac{\eta_{rel} d_p^2}{18}$$

Darcy equation $$\partial_t \rho + \nabla \cdot \left(\rho \frac{\kappa}{\mu} (\nabla p - \rho \mathbf{g}) \right) = 0$$

- Particle drag force
- Unconstrained particle aggregate (floc) diameter: $\boldsymbol{d_p}$ **= 30 µm**
- A cubic law for the settling velocity u_p in terms of the fracture aperture δ (**α = 3/2**). Note for δ = 0.1 mm, a linear law (**α = 1/2**)

Implementation

Three governing equations have been solved with a staggered scheme

Sodium cation transport
- Diffusion

Smectite expansion
- Smectite diffusive transport
- Herschel-Bulkley rheological model
- Shear resistance due to non-expansive gel below CCC

Water flow
- Advection (Darcian flow)
- Sedimentation model

Coupled approach

COMSOL MULTIPHYSICS®

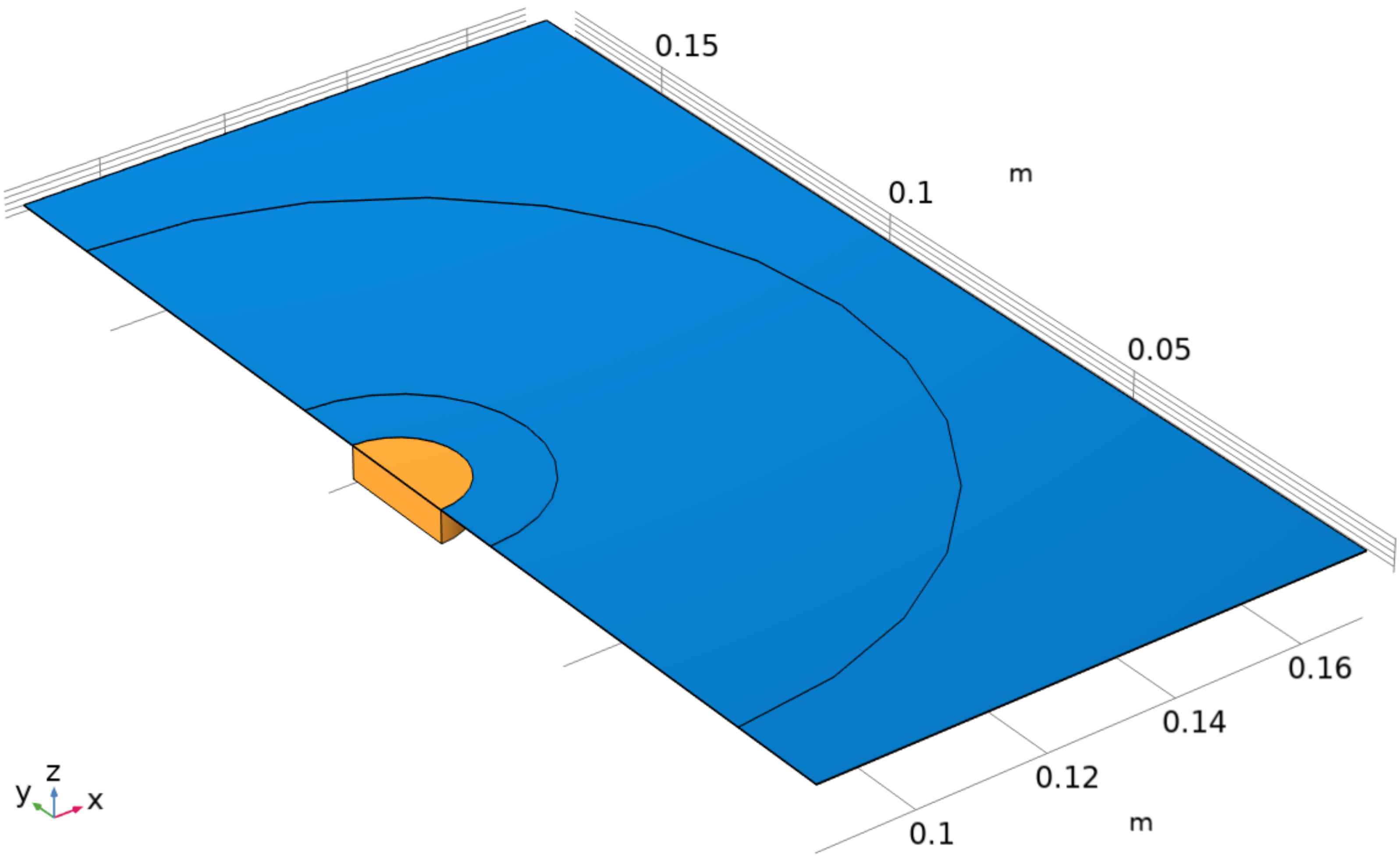
✓ High adaptability

✓ Easy implementation

✓ Computational efficiency

Implementation

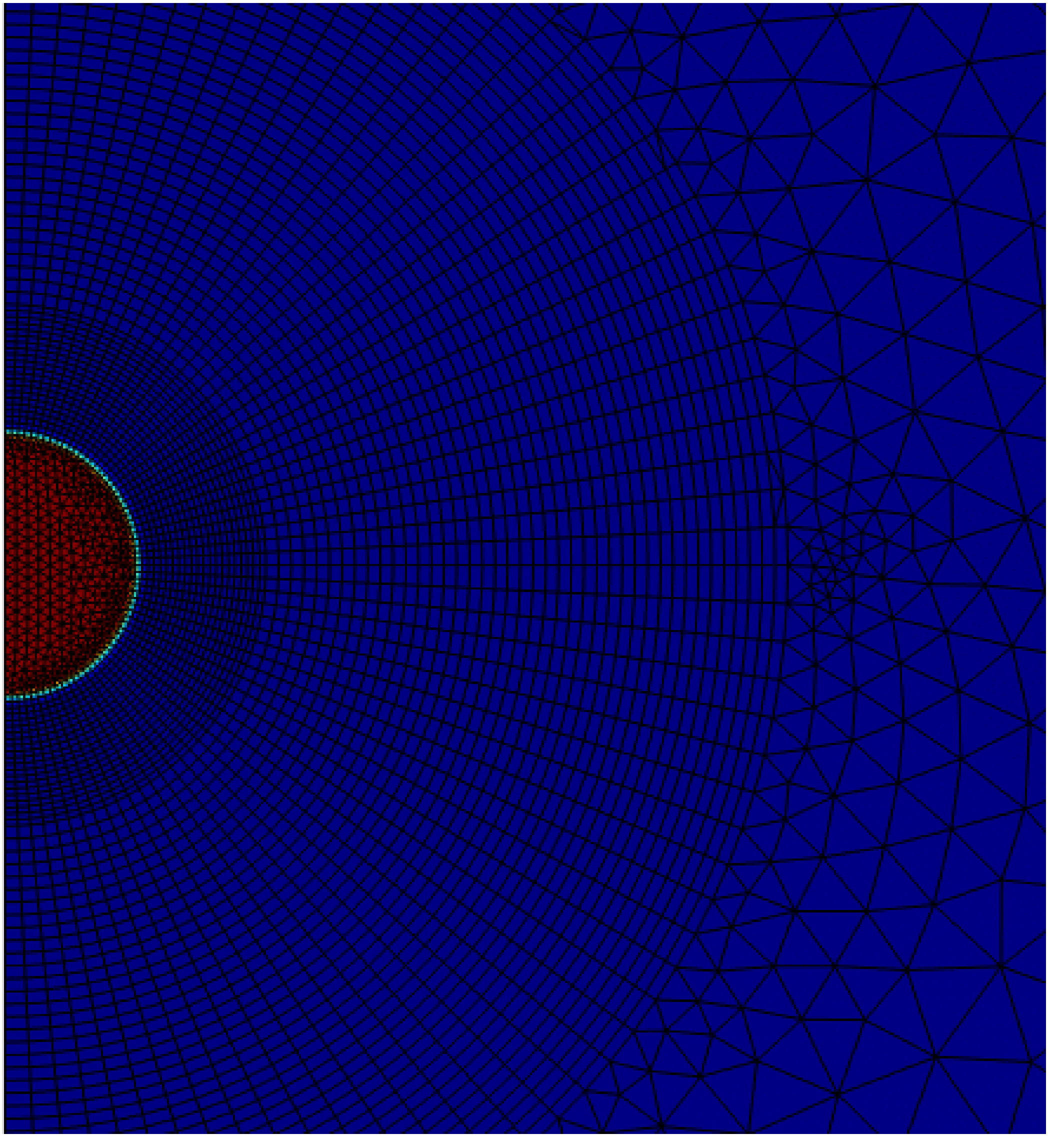
- 3D model of a bentonite pellet intersected by a fracture
  (a quarter of the domain)



Implementation

- A domain decomposition with a prescribed motion at the rim (**moving mesh**) had been developed in order to consider wall friction as a boundary force (Gauss theorem)

- Range of number of elements: 15k – 180k



Validation cases

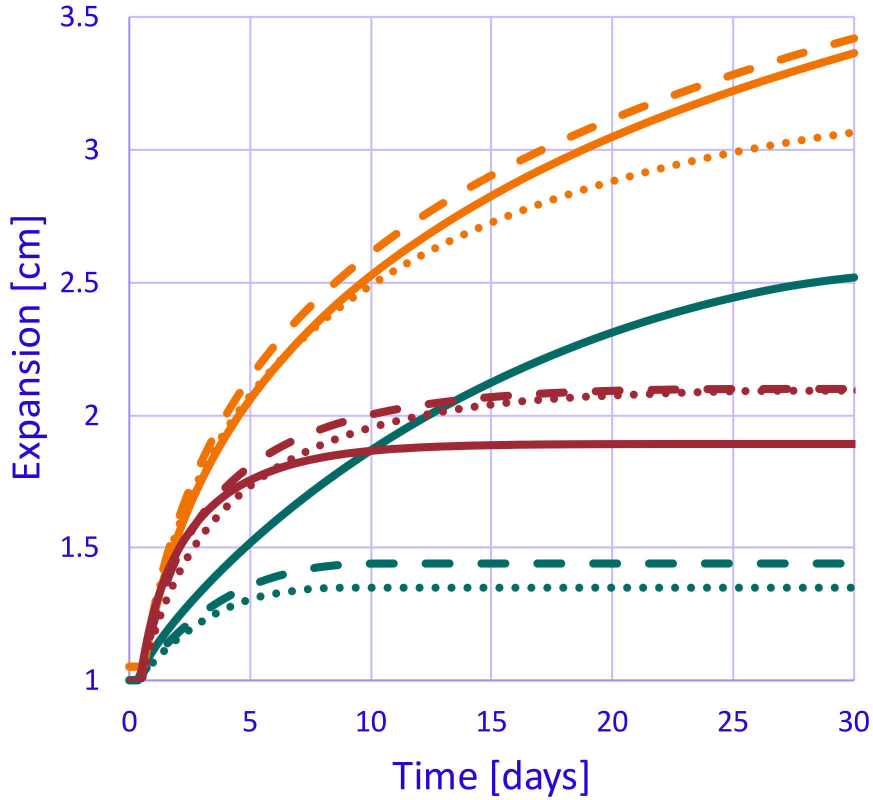
The **model is validated** with relevant **experimental data of small-scale tests** including different bentonite, pellet volumes, fracture apertures, initial dry densities, slopes, and flow rates.

Ref.	Case	Bentonite type	Dry density [kg/m³]	Initial radius [m]	Water inlet velocity [m/s]	Fracture aperture [mm]	Fracture slope (º)	Duration [d]
[1]	Schatz(2017)#2a	**MX-80**	1400	0.01	0	0.1	**0**	30
	Schatz(2017)#2b	**MX-80**	1400	0.01	0	0.1	**45**	30
	Schatz(2017)#2c	**MX-80**	1400	0.01	0	0.1	**90**	30
[2]	Ciemat(2022)#14	**Nanocor**	1400	0.0095	0	**0.1**	90	30
	Ciemat(2022)#15	**Nanocor**	1400	0.0095	0	**0.45**	90	30
	Ciemat(2022)#16	**Nanocor**	1400	0.0095	0	**0.36**	90	30
[3]	Hedström(2020)#1	**MX-80**	1420	**0.0175**	$2.96 \cdot 10^{-5}$	0.1	90	63
	Hedström(2020)#2	**MX-80**	**1420**	**0.01**	**$2.96 \cdot 10^{-5}$**	0.1	90	63
[4]	Schatz(2020)#5	**MX-80**	**1100**	0.01	**$5.60 \cdot 10^{-5}$**	0.1	90	63

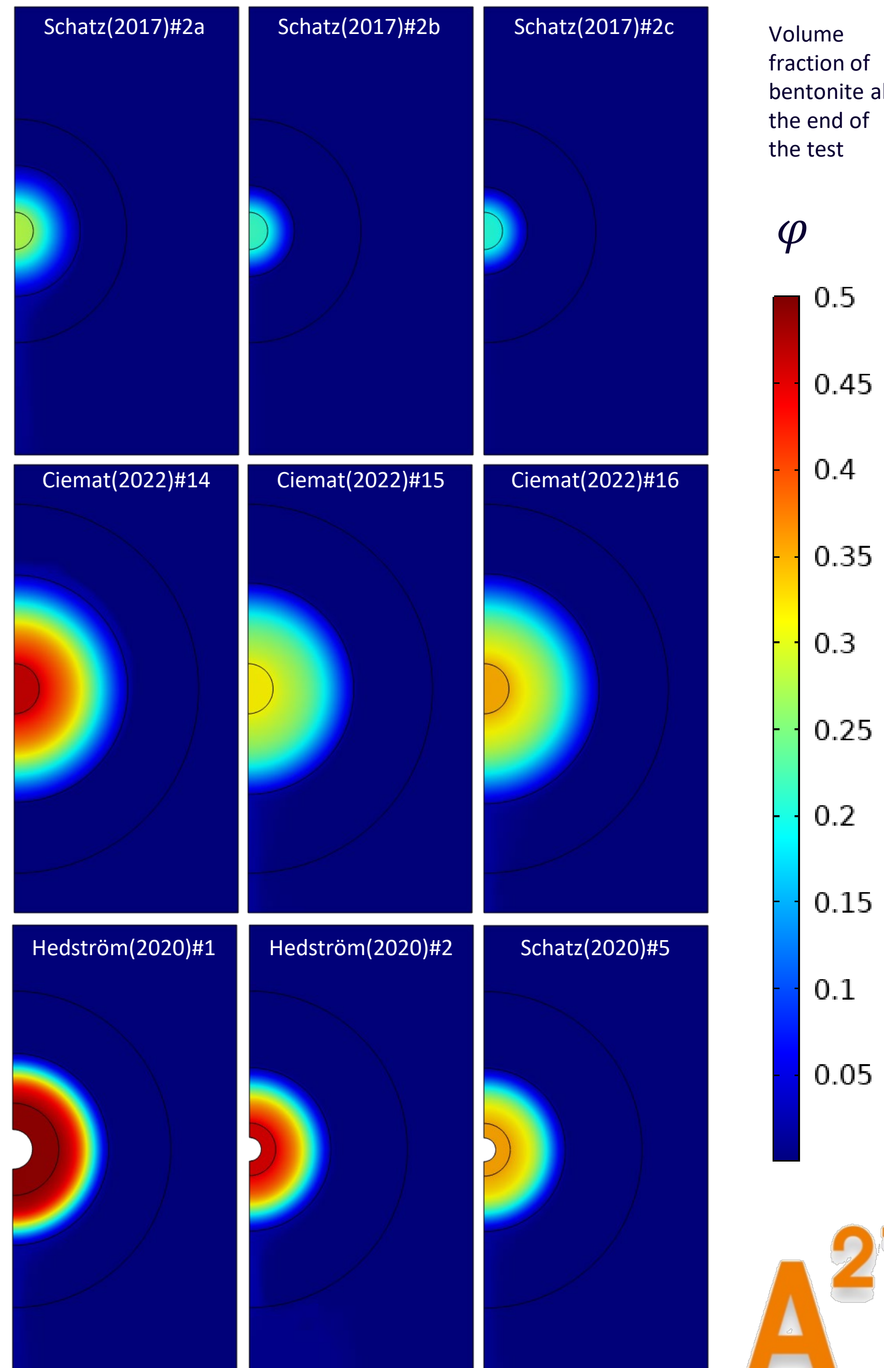
Infiltration water (all tests) → $[Na^+]$ = 1 mM

[1] Schatz and Akhanoba (2017). Bentonite buffer erosion in sloped fracture environments. Posiva 2016-13
[2] Ciemat (2022). Benero: Bentonite Erosion project
[3] Hedström (2020). Empirical Assessment of Chemical Erosion. Clay Technology AB.
[4] Schatz (2020). Empirical Assessment of Chemical Erosion. Task 3.

Results

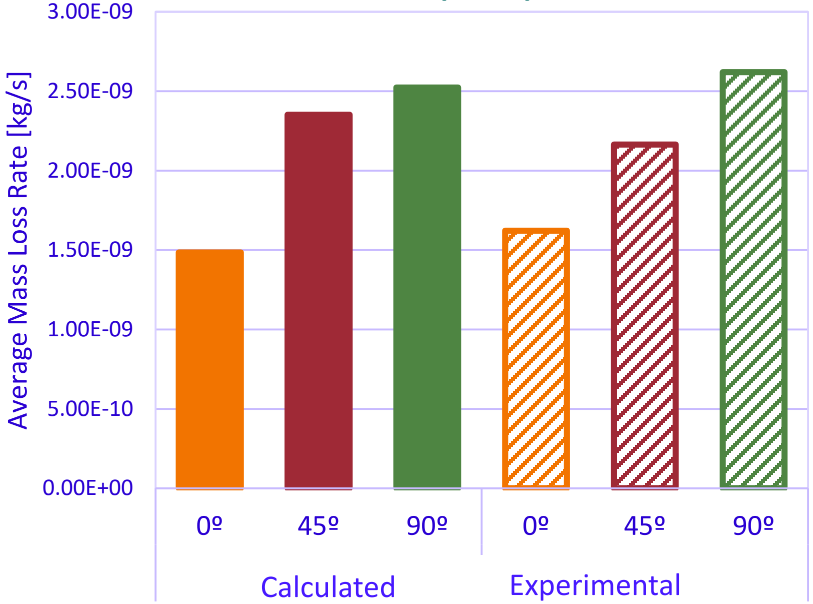


Fracture slope:	0º	Schatz(2017)#2a
	45º	Schatz(2017)#2b
	90º	Schatz(2017)#2c
Fracture apertura:	0.1 mm	Ciemat(2022)#14
	0.36 mm	Ciemat(2022)#16
	0.45 mm	Ciemat(2022)#15
Dry density | Initial pellet radio:	1420 kg/m3 | 1.75 cm	Hedström(2020)#1
	1420 kg/m3 | 1 cm	Hedström(2020)#2
	1100 kg/m3 | 1 cm	Schatz(2020)#5

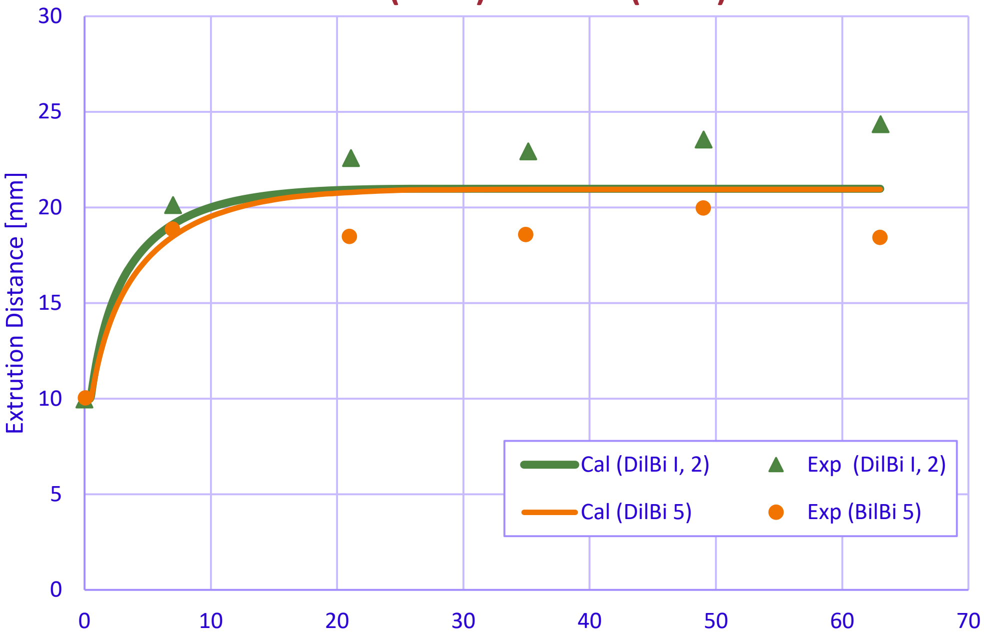


Results

Schatz(2017) tests



Hedström(2020) & Schatz(2020) tests



	Case	Expansion radius [cm]		Extruded mass [g]		Eroded mass [g]	
		Experimental	Calculated	Experimental	Calculated	Experimental	Calculated
*	**Ciemat(2020)#14**	--	3.37	--	0.34	--	0.00
	Ciemat(2020)#15	*3.65*	3.06	*0.89*	1.04	*0.54*	0.45
	Ciemat(2020)#16	*3.77*	3.42	*0.87*	1.04	*0.28*	0.18

** Experimental data are no yet available (test in progress)*

Conclusions

- The **model for bentonite expansion and erosion has been** developed in **COMSOL Multiphysics** due to its high adaptability, easy implementation and computational efficiency.
- **Sodium cation transport**, **smectite expansion and fracture flow** have been coupled.
- A domain decomposition with a prescribed motion at the **bentonite-water** (**moving mesh**) has been developed in order to consider **wall friction as a boundary force** (Gauss theorem).
- The **sedimentation model**, although at a preliminary development stage, has yielded promising results in a wide range of scenarios.
- **Next step**: **upscaling** to predict the expansion and erosion of bentonite in fracture under repository conditions.

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