WP 5: Conceptual and mathematical models

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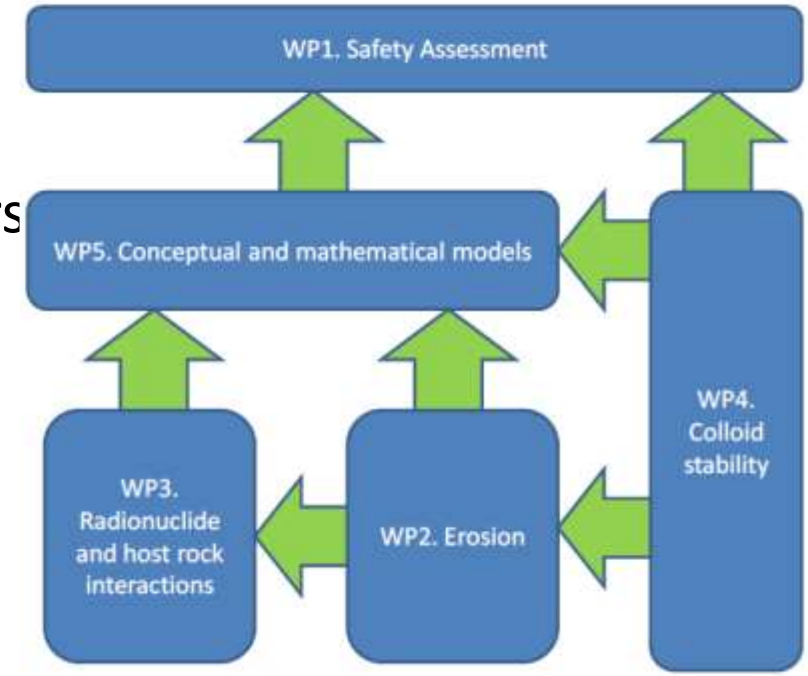
The course of events

2011	Objectives at the outset
2012	Review of models in the beginning
early 2013	Early advances
late 2013	Definition of benchmark
early 2015	Scaling from small-scale to full-scale
late 2015	The current uses in Safety Cases based on BELBaR-work

Objectives at the outset– 1/2

From DoW

- **Validate** and advance the **models** for predicting
  - mass loss of clay in dilute waters and clay colloids generation in special and
  - clay colloids facilitated radionuclide transport.
- **Formulate data needs** from other WP's
- **Use** the overall **understanding** in the safety assessment formulations **in WP1**



Objectives at the outset– 2/2

From DoW

- Conceptual modelling
  - reason dominant processes,
  - identify and reason relevant parameters and
  - articulate the data needed to implement new aspects.
- Mathematical and numerical modelling
  - validate models by predicting small-scale experiments (WP2-4)
    - reason scaling using conceptual understanding
  - implement new features arising from elaborated conceptual models

Review of models in the beginning

State of the art of models -report

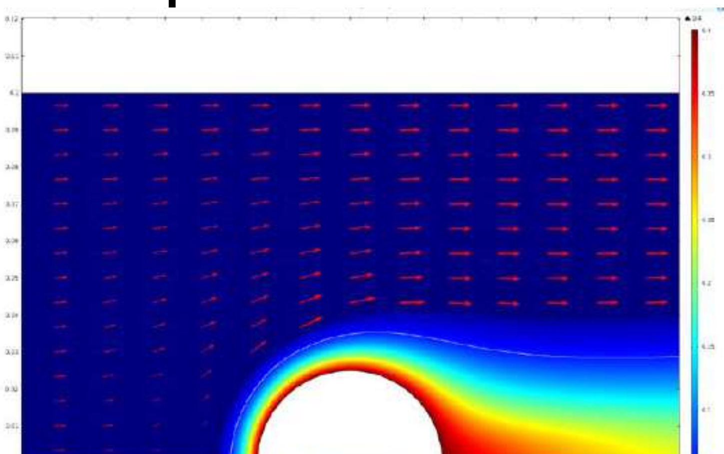
- Erosion of bentonite
  - baseline model by KTH
    - conceptual view
      - gel/sol behaviour and expansion
      - ion exchange and influence of divalent ions
      - friction in fractures
    - relevant parameters
      - viscosity of smectite gel/sol
      - forces on and between smectite particles
        - » gravity and buoyance
        - » changes in chemical potential
        - » attraction due to van der Waals
        - » repulsion due to electrical charges in and on smectite particles (DDL)
        - » friction
      - Debye length
    - numerical implementation
  - VTT modification of baseline model
    - simplification of some functional dependencies to enhance computational reproducibility
- Transport of bentonite colloids
  - Lagrangian implementation of particle migration
  - Colloid/nanoparticle interaction with stationary phase
  - heterogeneity of the domain – different assumptions tested with colloid breakthrough curves

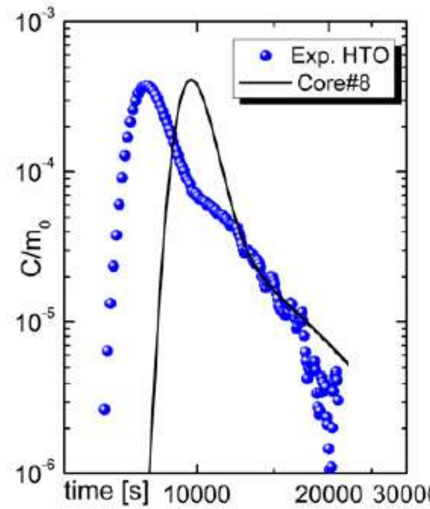
Early advances – 1/2

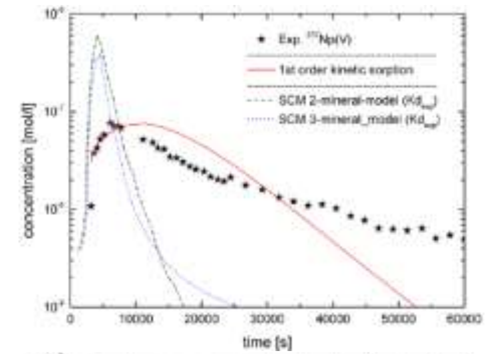
- Erosion of bentonite
  - simplifications sought for numerical model
  - mechanical model for SP presented (with stacking number as parameter)
  - development of alternative models for wetting and swelling at VTT
- Transport of bentonite colloids
  - systematic parameter studies need to be committed wrt transport of bentonite colloids

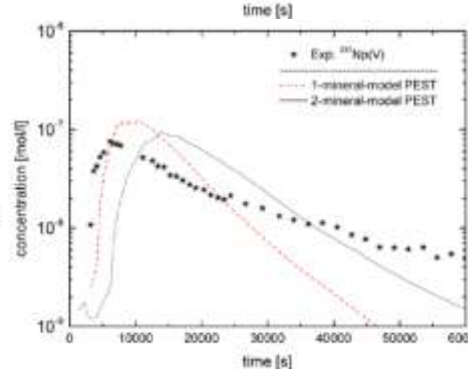
Early advances - 2/2

- Mismatch between computer simulations and experiments









Definition of benchmark – 1/3

- Justification of relevant processes and parameters accepted by participants missing

⇒BENCHMARK

- … in order to advance conceptual understanding AND
  - regarding which aspects?
  - make it more explicit

- … in order to validate numerical models
  - existing data?
  - new data?

Definition of benchmark – 2/3

- Aspects raised during and after the presentations

- Aspects selected for group discussions
  - central processes
  - accessory minerals
  - flocs
  - hysteresis
  - gravity

Definition of benchmark – 3/3

	PROCESSES	ACCESSORY MINERALS	FLOCS	HYSTERESIS	GRAVITY
GROUP 1	Swelling into fracture • measure details in the front • different apertures • in non-"sol forming" conditions • in "sol forming" conditions	Maybe not … just montmorillonite alone at this stage	Aren't they of part of buffer system?	Range of densities in which gel is table	Not doable

GROUP 2	• There are plenty of data available
	  • Rate of expansion
	  • Erosion rate
	• => FOCUS on swelling
	  • Maybe not in great details
		What is this actually about?
		• To include this we'd need to understand it better
			Not sufficiently well understood to be included into benchmarks	Data needed	Potentially important

GROUP 3	• Keep it limited • Expansion -> rate • (erosion -> rate) • 2bv~0.1 mm • NaMt • Tabletop • Low salinity 1 mM NaCl • No flow • -> Experiment -> upscaling the geometry • Expansion -> erosion -> geometry upscaling	Not to be considered in benchmarks	This is conceptual uncertainty - > This is question for modellers!	Not to be considered in benchmarks -> premature	We have too little data for benchmark -> premature

Scaling from small-scale to full-scale – 1/5

Ability to predict the experiments?

- two-region model developed
  - ”high resolution of rim only” -model
  - can be further simplified
  - impact of

    ”old” full resolution model → simplified two-region model:

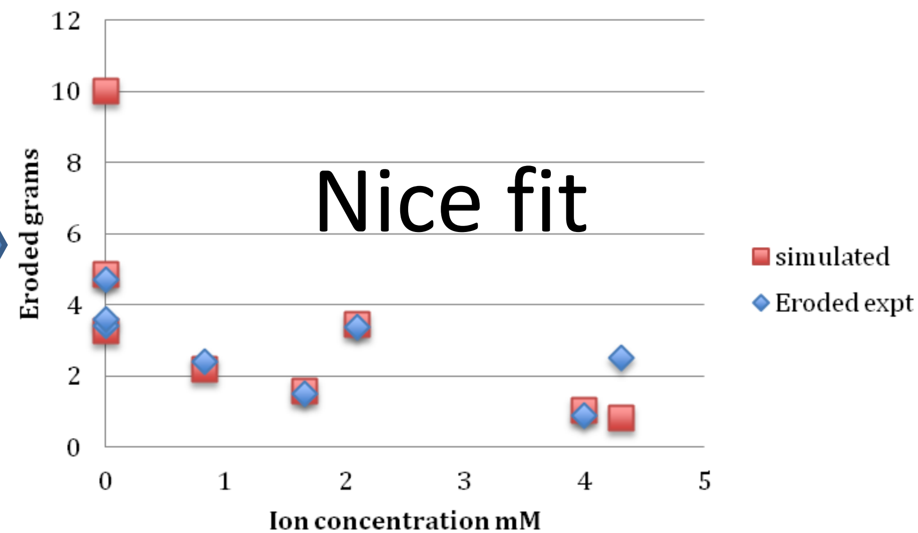
    mass loss ↓(factor of 1.5…5)

    ⇒r_{RIM}↑ (factor of 5…30))

- validation with 1:88 tests
  - far from satistactory

    ⇒ assume:

    - flocs move with water
    - & $\phi_{@rim}$=const



Scaling from small-scale to full-scale – 2/5

Uncertain effects of factors

- longer rim
  - see next slides
- smectite → bentonite
- migration of flocs under gravity
  - boundary estimate: loss of clay as agglomerates at rim restrained by agglomerate migration
- others???

Scaling from small-scale to full-scale – 3/5

Simplified two-region model

velocity [m/s]	**1E-07**	**1E-06**	**1E-05**
velocity [m/a]	*3*	*32*	*315*
Mass lost [kg]	140	148	172
Eroded mass [kg]	7,6	22	144
penetration depth [m]	34,2	32	14,7
time [a]	10000	10000	10000
mass loss [g/(m^2 a)]	**34**	**107**	**1 471**

← depends on velocity (not evident in experiments)

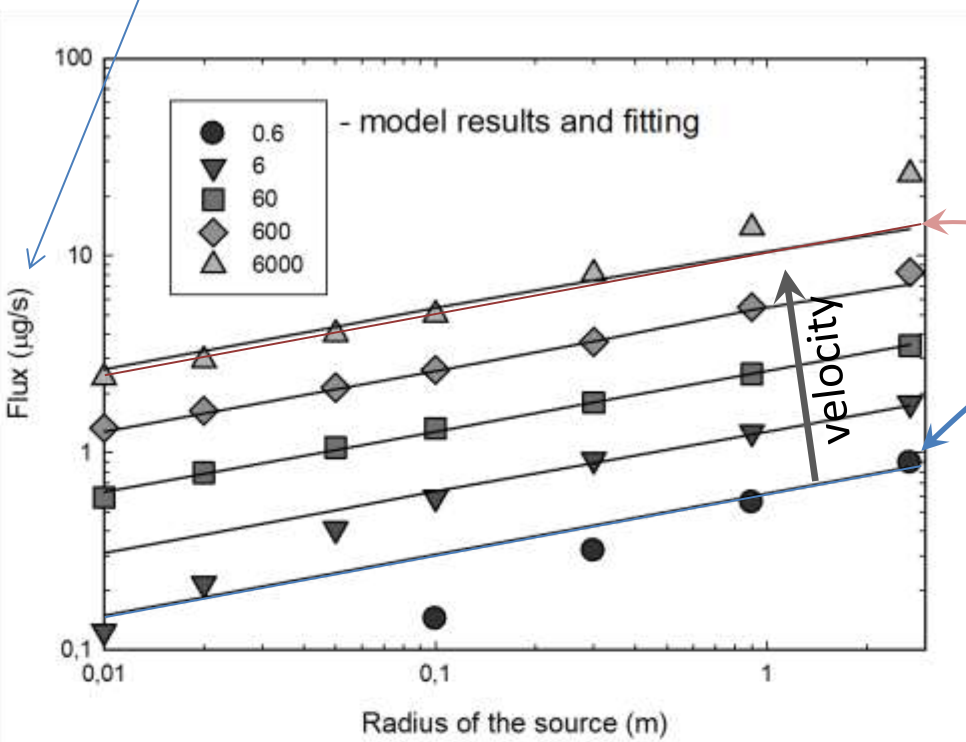
Scaling from small-scale to full-scale – 4/5

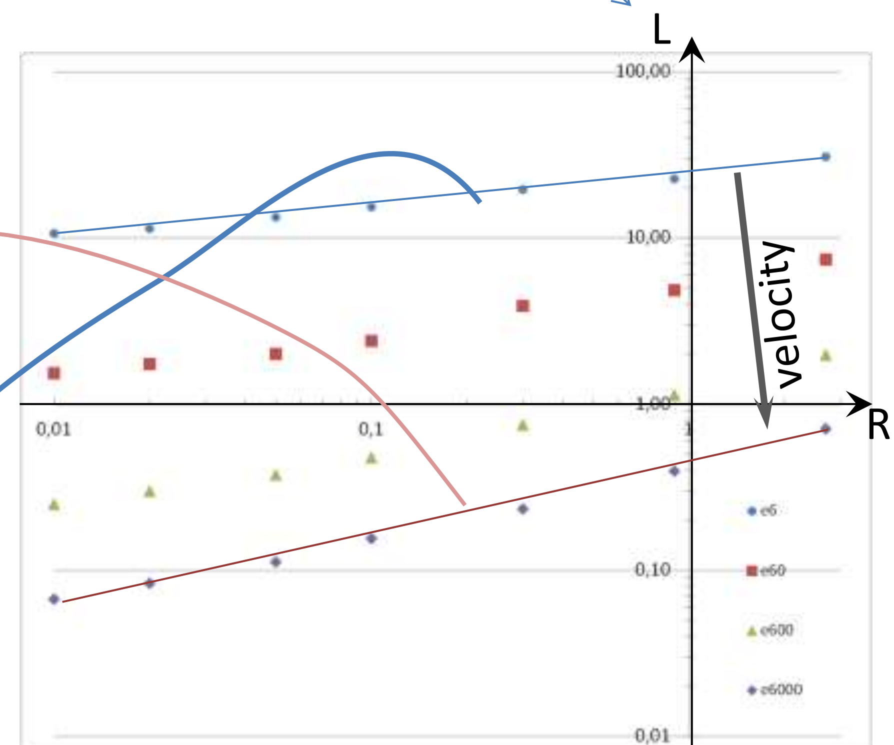
"old" full resolution model → simplified two-region model in 1:88

"Detailed view" into intermediate scales

– giving higher estimates of mass loss

– giving lower estimates of rim location, L

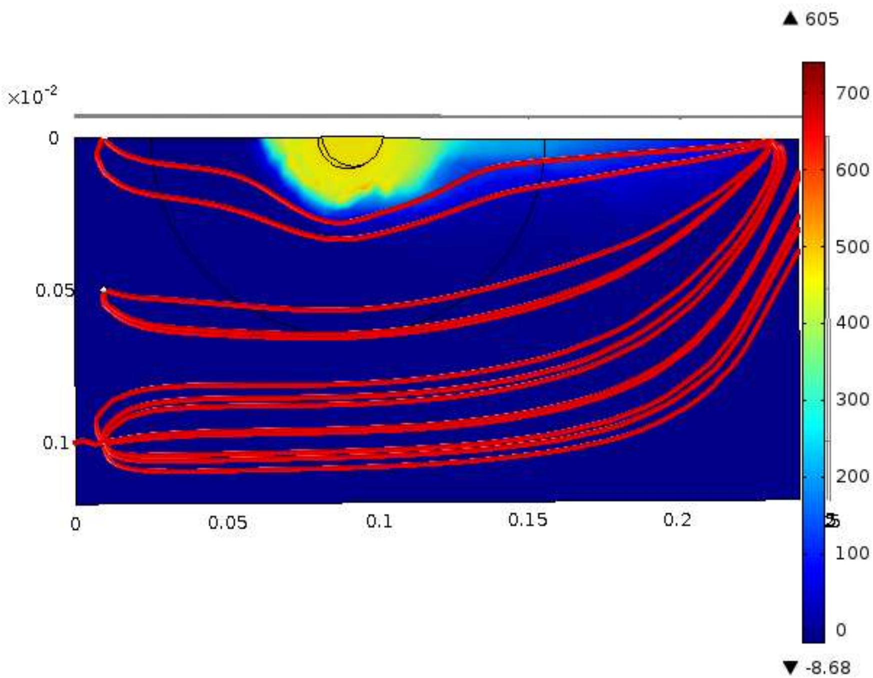


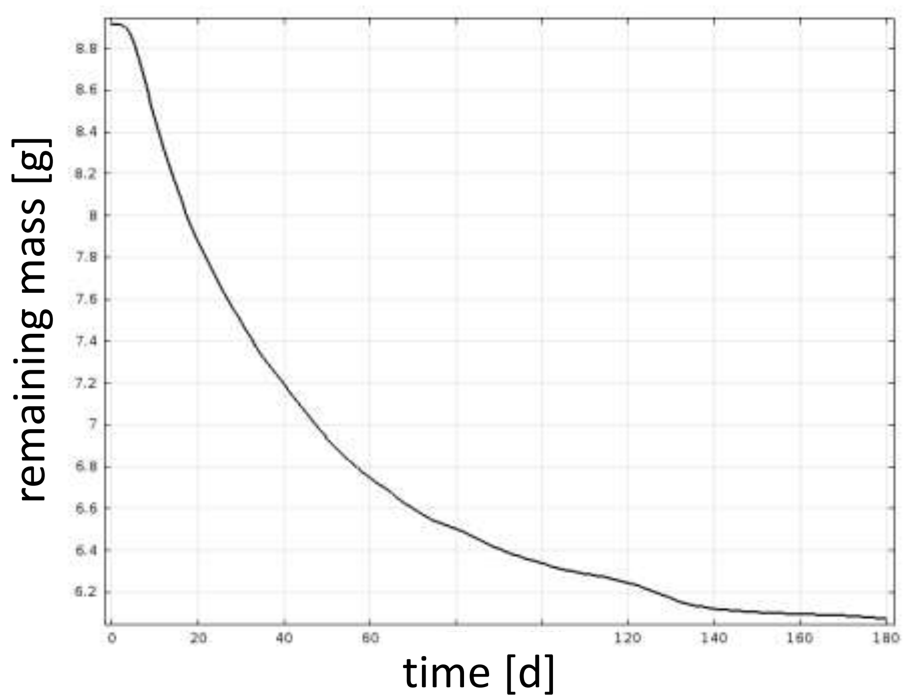


Scaling from small-scale to full-scale – 5/5

Alternative model development not finished …

- 3D!!!
- Water can flow through the colloid mass (Brinkman flow)
- Stokes-Brinkman equations: Stokes + effect of porosity





The current uses in Safety Cases based on BELBaR-work– 1/3

Against DoW

- **Validate** and advance the **models** for predicting?
  - mass loss of clay in dilute waters
    - nice match in 1:88-scale
    - bounding estimates in 1:1-scale
  - clay colloids facilitated radionuclide transport
    - dd
- **Formulate data needs** from other WP’s
    - data for penetration into fracture and erosion for NaMt
    - erosion dynamics for bentonite
    - strength of structure at rim
- **Use** the overall **understanding** in the safety assessment formulations **in WP1**
    - bounding estimates for mass loss of clay in dilute waters

The current uses in Safety Cases based on BELBaR-work– 2/3

Against DoW

- Conceptual modelling
  - reason dominant processes
    - swelling, flocs migration, gravity
  - identify and reason relevant parameters
    - initiated in benchmark but not agreed to finish
  - articulate the data needed to implement new aspects
    - see previous slide **Formulate data needs**
- Mathematical and numerical modelling
  - validate models by predicting small-scale experiments (WP2-4)
    - reason scaling using conceptual understanding
      - ability to perform bounding estimates
  - implement new features arising from elaborated conceptual models
    - Done

The current uses in Safety Cases based on BELBaR-work – 3/3

- Bounding estimates using numerical simulation methods developed in BELBaR
- These estimates to justify the assumptions used in Safety Cases

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