Flow and reactive transport modeling in radioactive waste repositories

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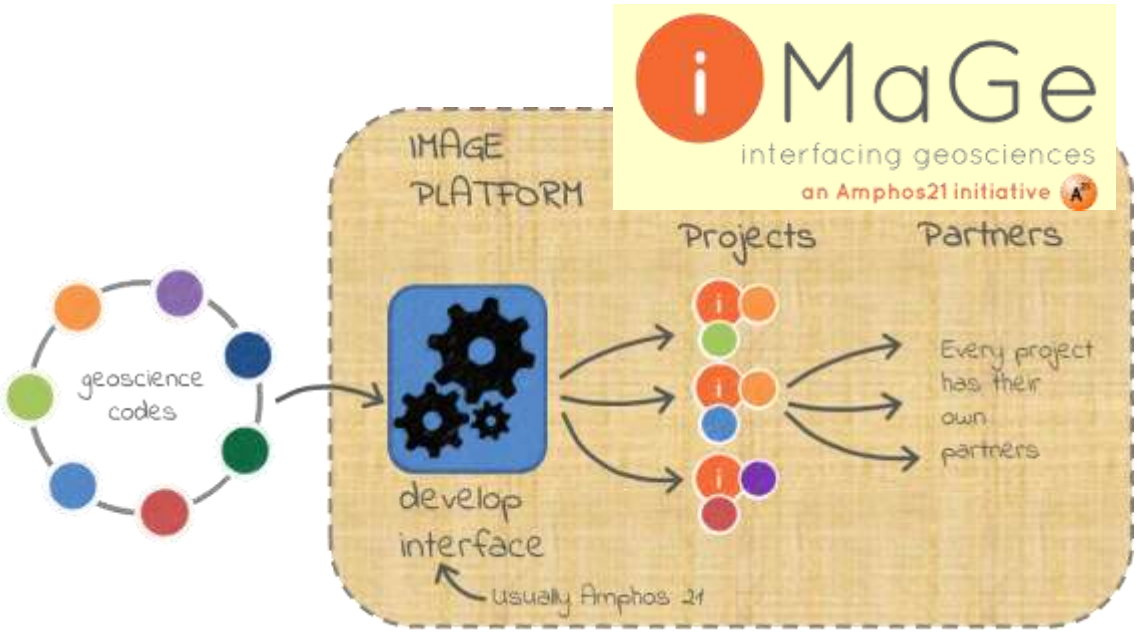
Outline

- Modeling tools and relevant projects
- Comsol example: groundwater modeling of SFR repository
- iDP example: grout degradation in a DGR
- iCP example: chemical evolution of a HLW cell
- Summary

Modeling tools and relevant projects



Codes

- COMSOL
- DARCYTOOLS
- PHREEQC
- PFLOTRAN
- etc.

1 application case with COMSOL and 2 application cases with interfaces

COMSOL

idarcytools
pflotran

icomsol
phreeqc

Projects

1. Groundwater modeling of SFR repository (SKB) → COMSOL
2. Grout degradation of a DGR (Forsmark, SKB) → iDP
3. Chemical evolution of a HLW cell (ANDRA) → iCP

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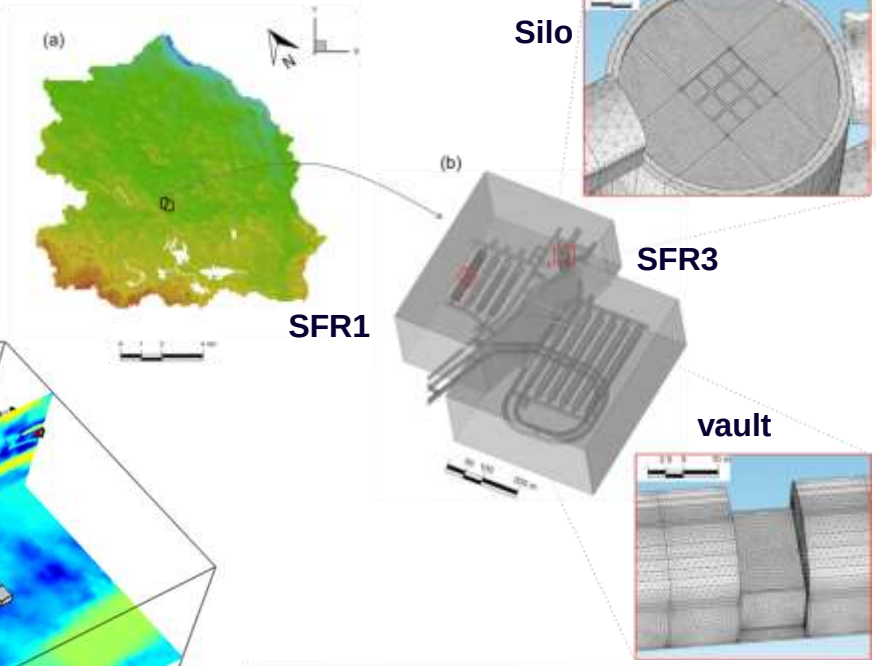
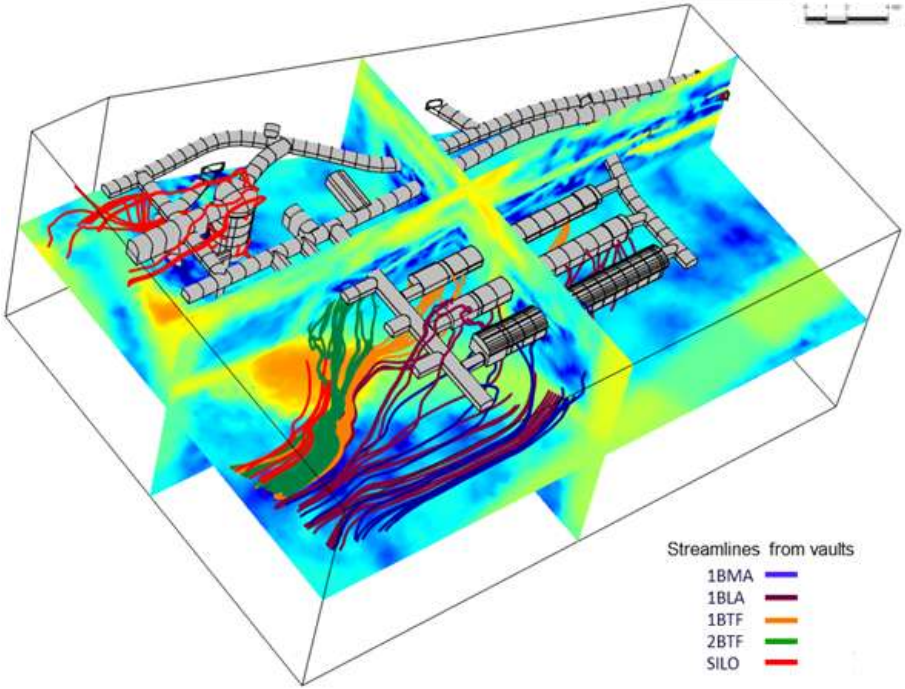
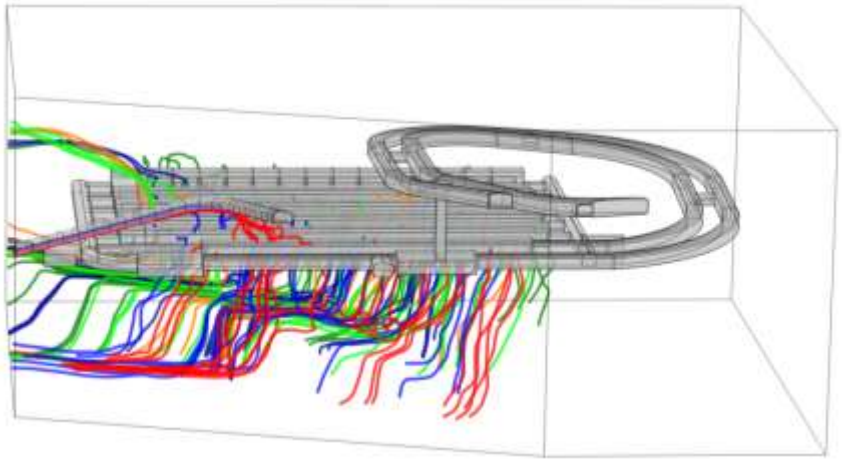
1. Groundwater modeling of SFR repository (SKB, Forsmark)

10,748,580 (SFR1) and **11,548,320** (SFR3) tetrahedral quadratic finite elements





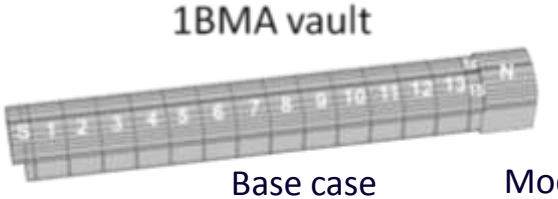
SFR1. Groundwater streamlines leaving the individual vaults under degraded plugs scenario

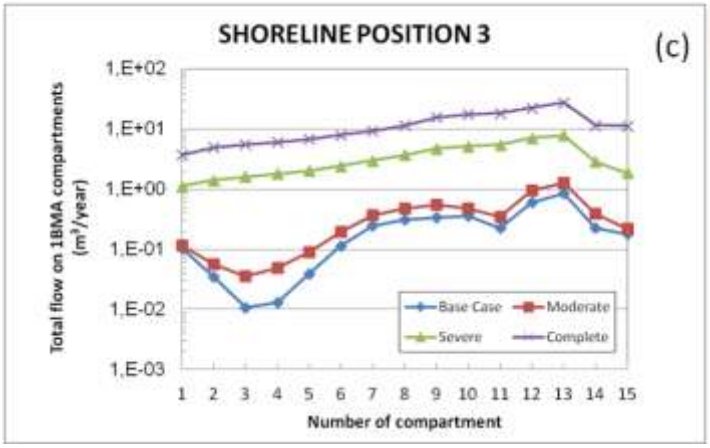


SFR3. Groundwater streamlines leaving the individual vaults under complete concrete degradation

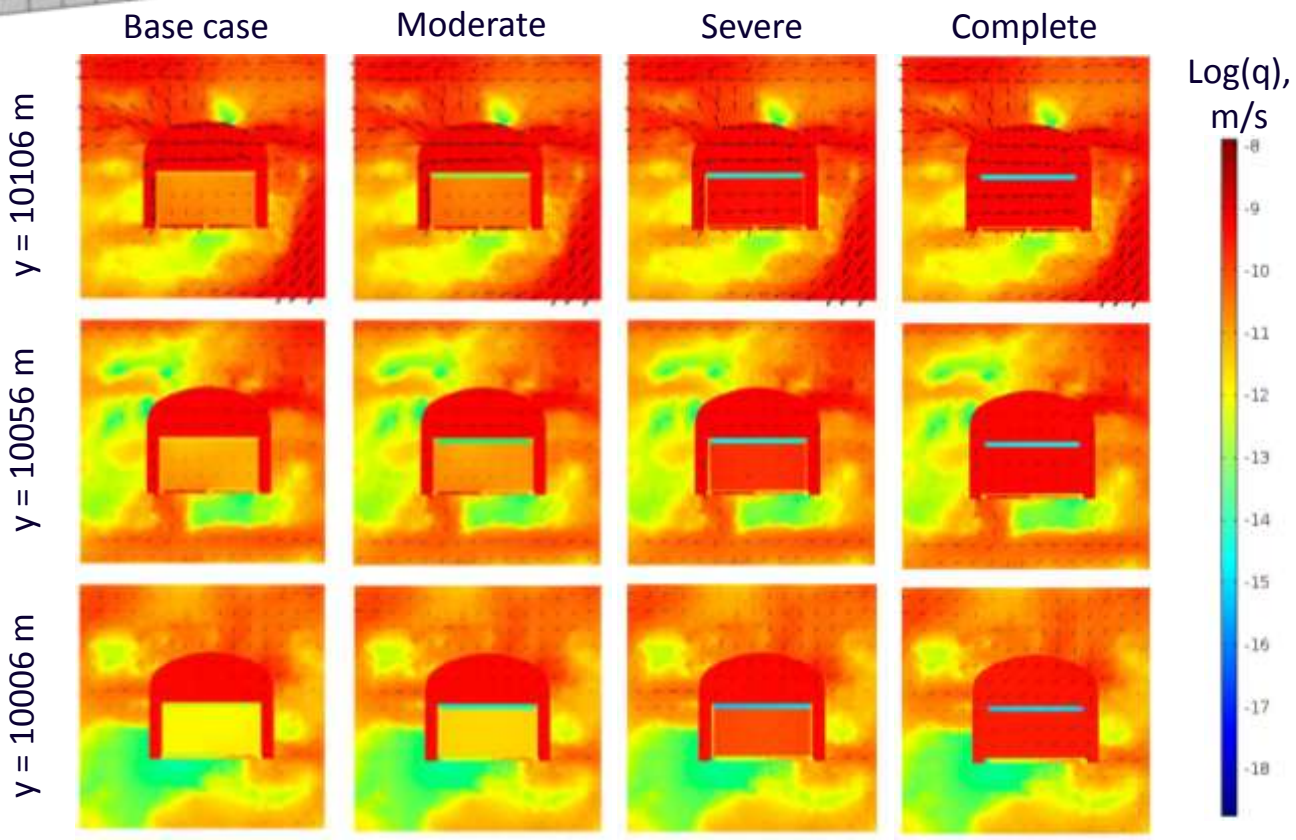
Flow and transport on the vault subscale. Elements degradation

Degradation of inner and outer walls of 1BMA vault





Flow through waste compartments



Velocity field at 3 cross sections of the 1BMA vault

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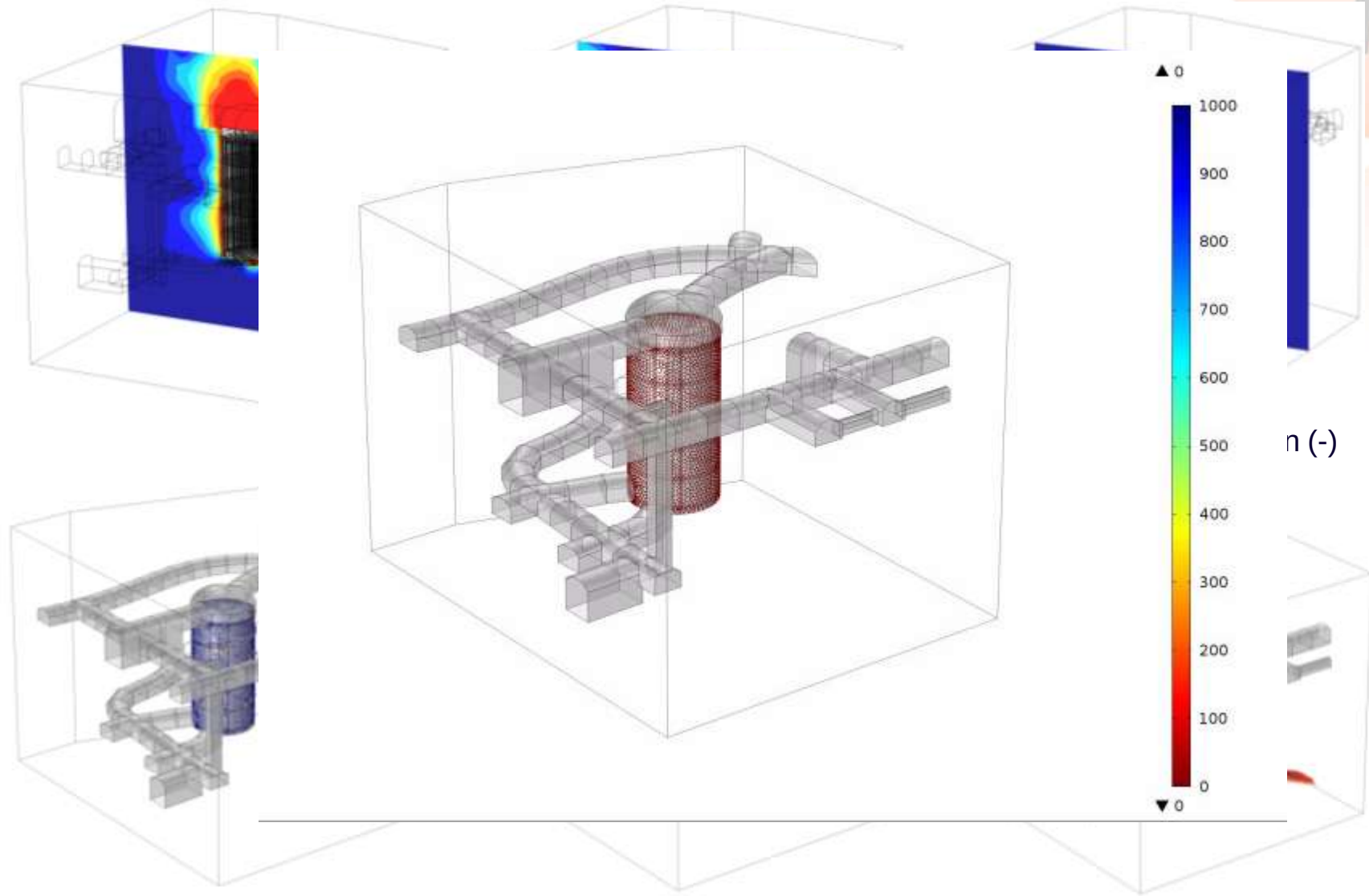
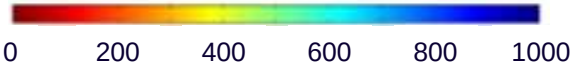
Flow and transport around the Silo

Shoreline position 1 Shoreline position 2 Shoreline position 3





Time, years

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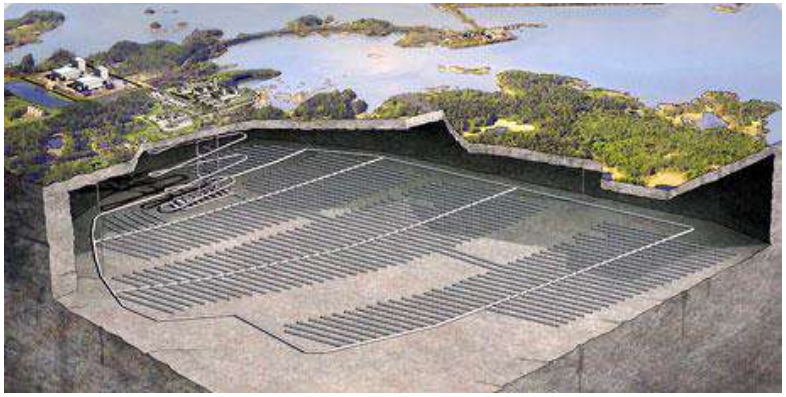
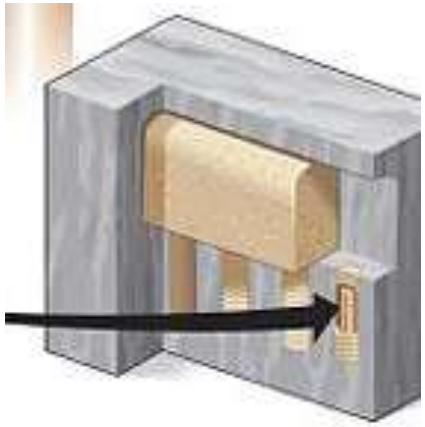
2. Grout degradation in a DGR: SR-site (SKB, Forsmark)

- **SKB** is planning the construction of a **DGR** for disposal of spent nuclear fuel



- SKB concept (**KBS-3**) is based in a multi-barrier system, including compacted bentonite surrounding the spent fuel canisters



During the construction of the tunnels, water-conducting fractures will be sealed with cement-based grout. After closure of the tunnels, this could lead to the formation of **hyper-alkaline (high pH) water, that can be detrimental for the stability of bentonite**.

Objective: to evaluate the possibility of hyper-alkaline water plume development, and **the risk of reaching repository depth**

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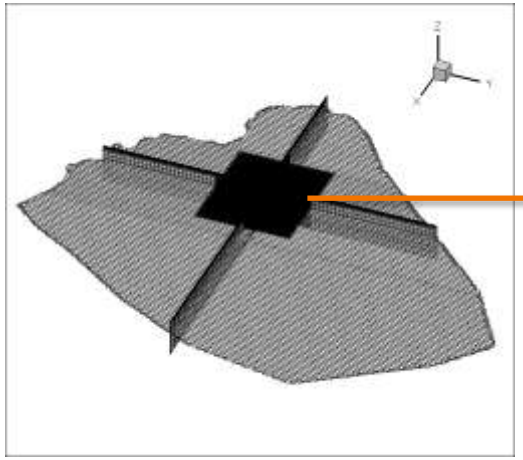
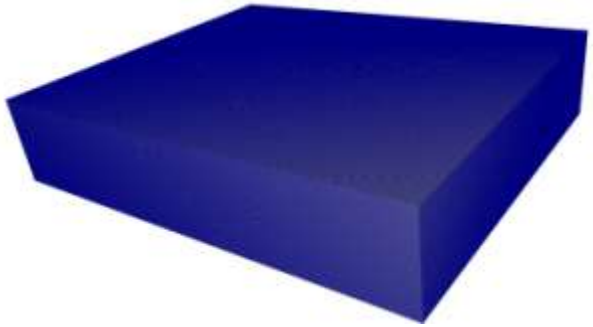
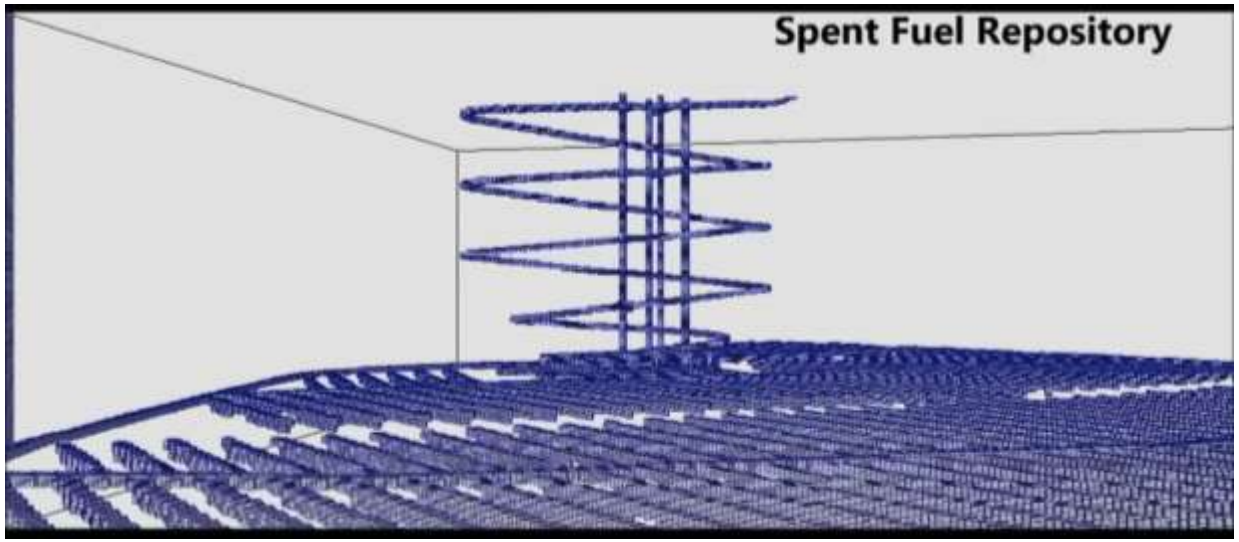
Grout degradation in a DGR: domain discretization



Flow simulation grid in **DarcyTools** (**105.044.948** cells)



Reactive transport grid in **PFlotran** (**102.394.896** cells; Cell size: 4m x 4m x 2m)



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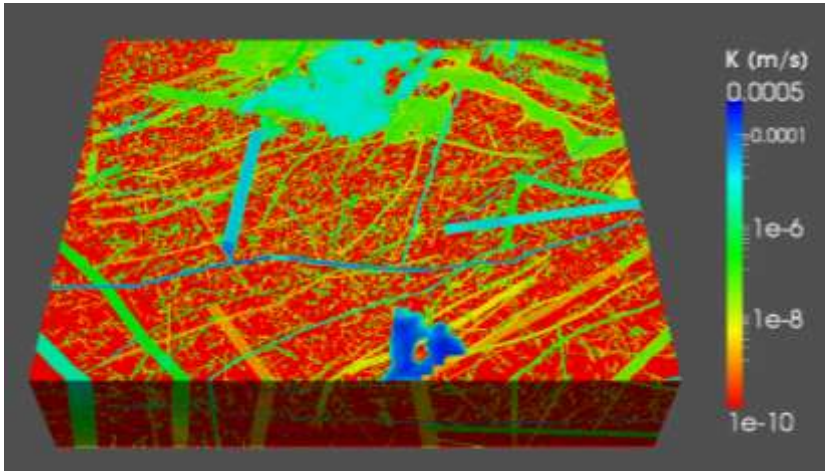
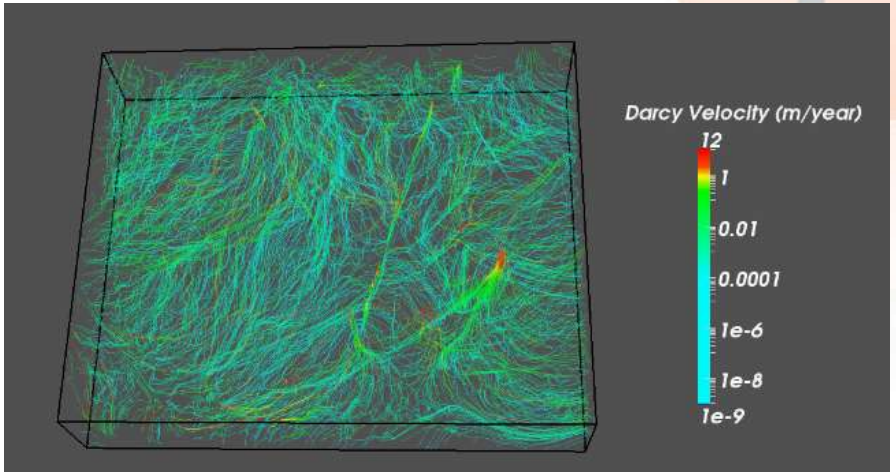
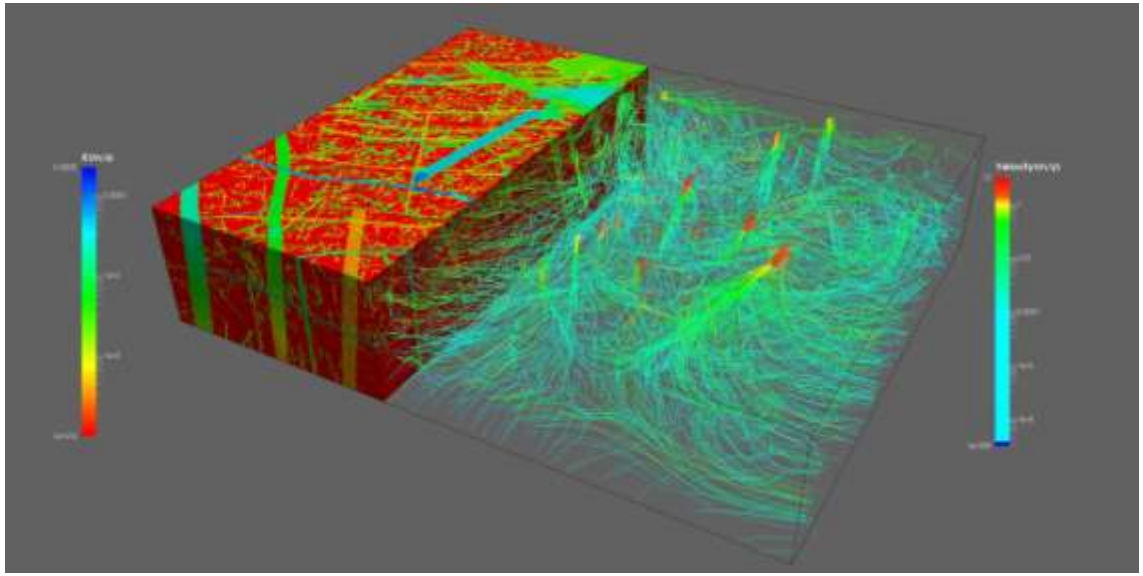
Flow results: Darcy velocity field (Darcy Tools)

Hydraulic conductivity field calculated with DarcyTools



Steady state velocity field calculated with DarcyTools





Simulated flow responds to fracture distribution

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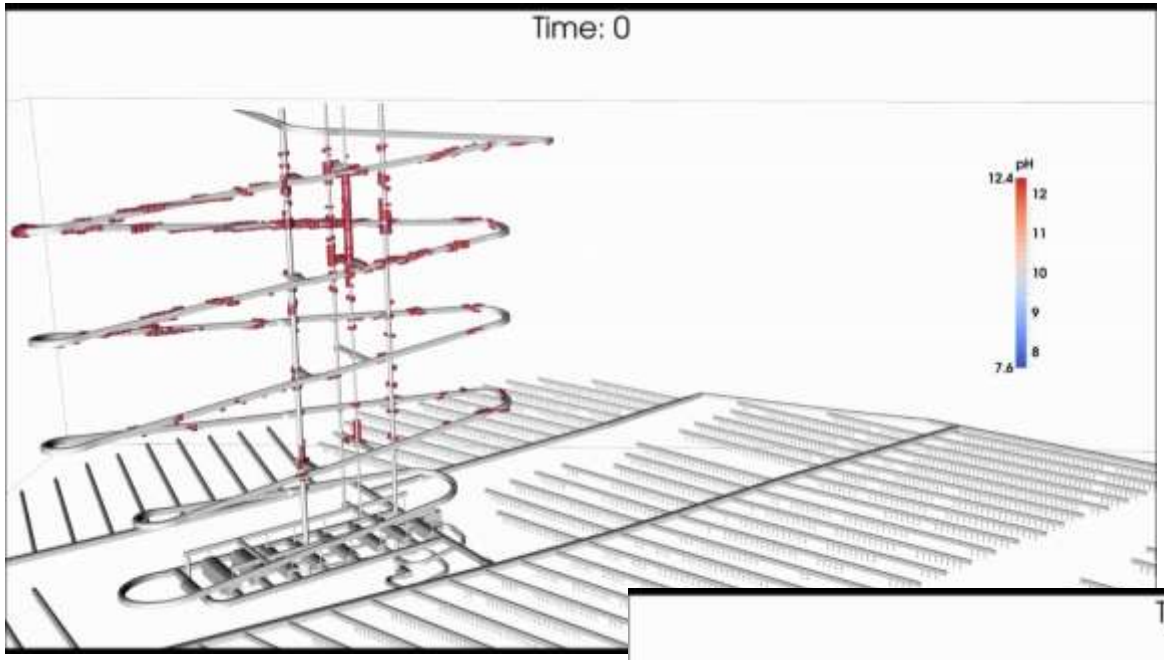
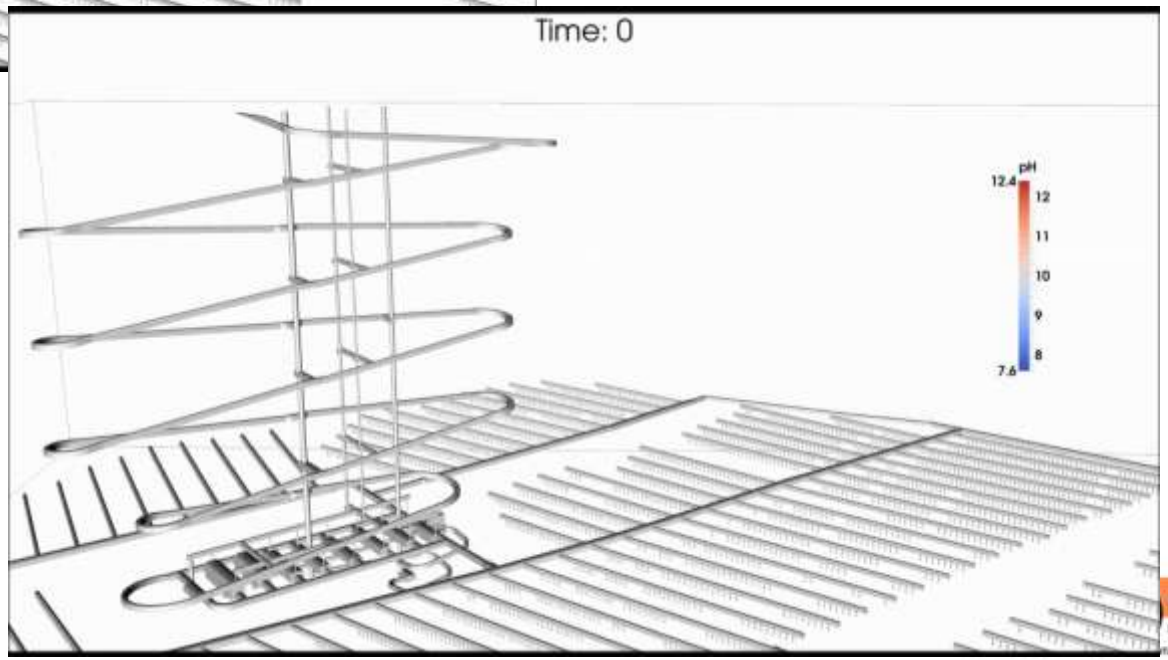
Reactive transport results (PFLOTRAN): pH

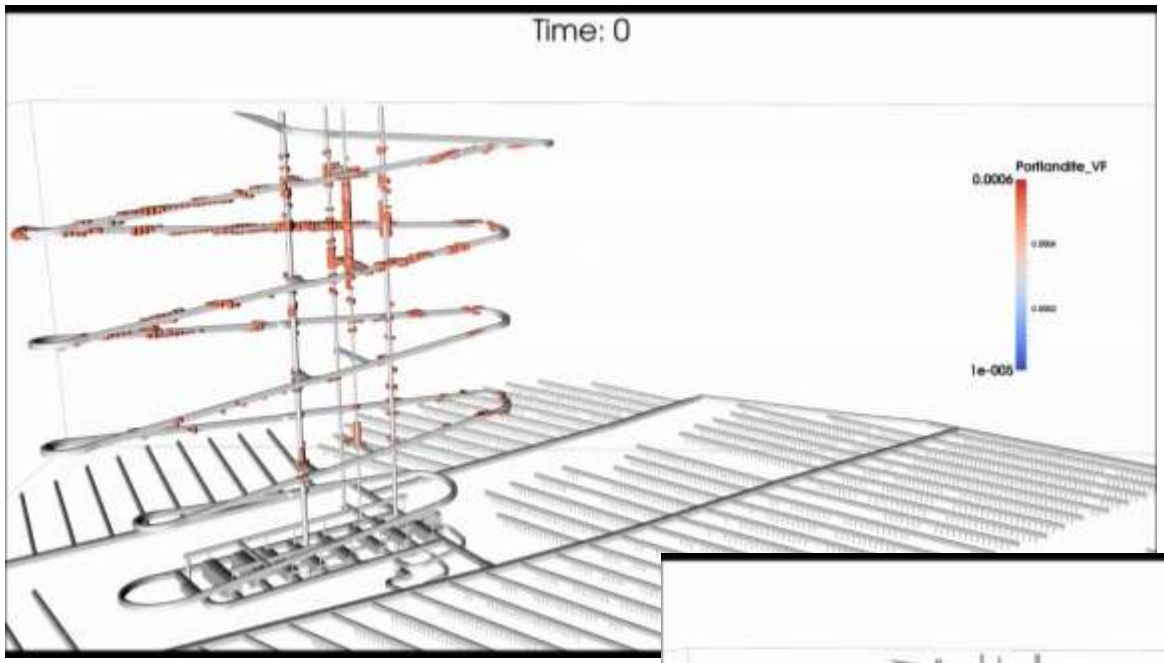


pH > 7.6

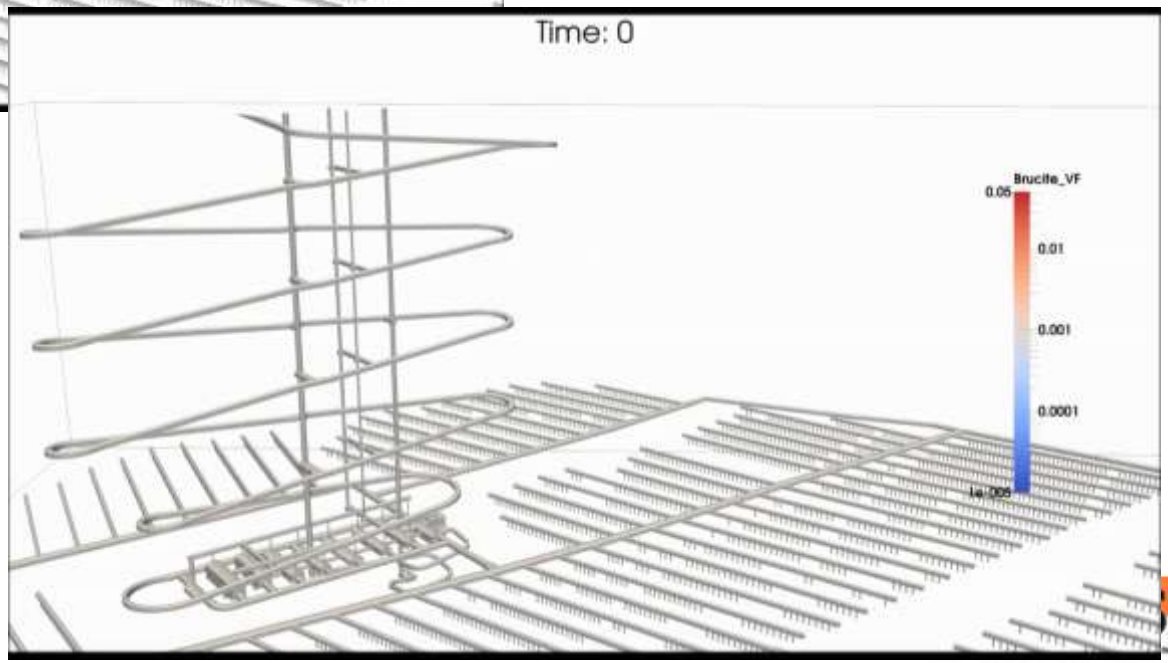


pH > 11

Reactive transport results (PFLOTRAN): Portlandite & Brucite

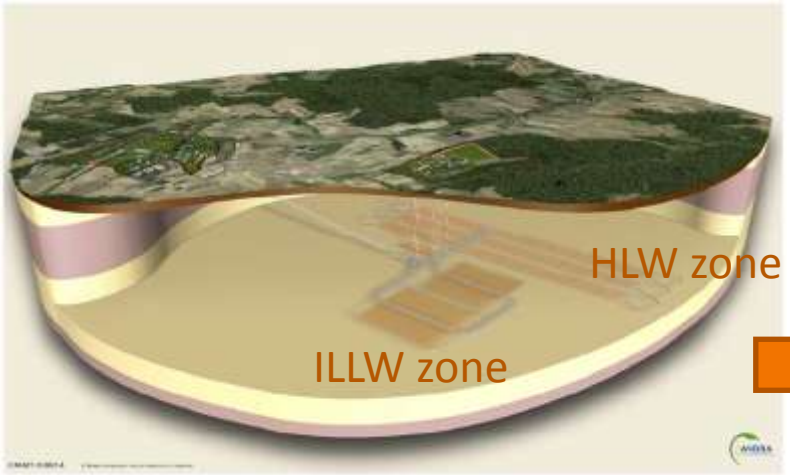


Portlandite dissolution

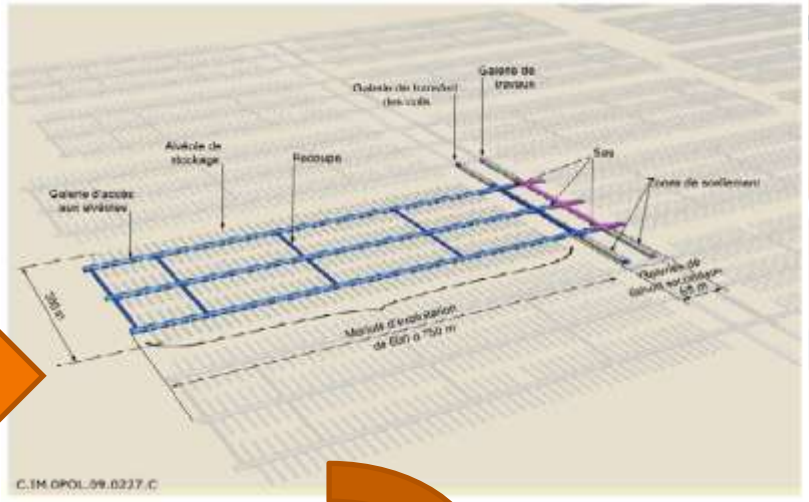


Brucite precipitation

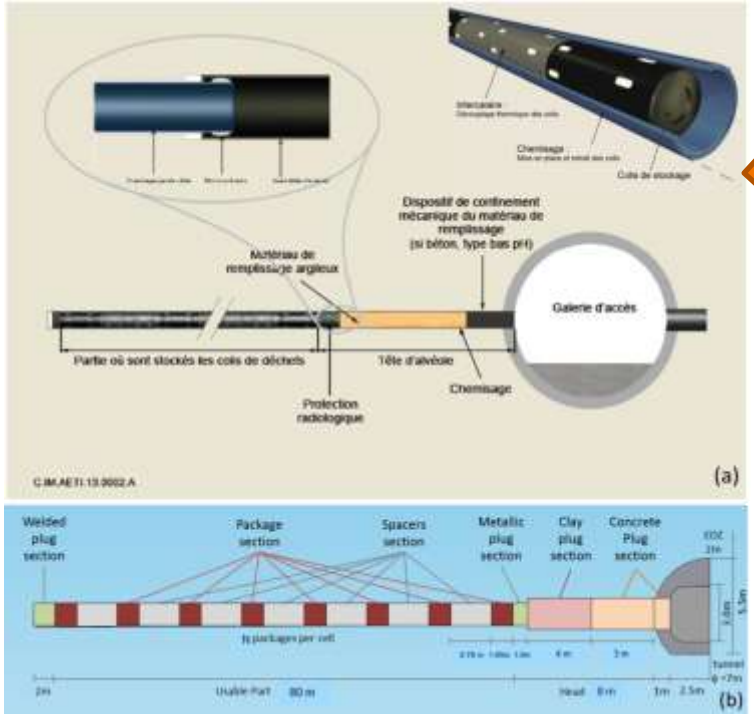
3. Chemical evolution of a HLW cell (ANDRA)



View if the deep disposal project (CIGEO)



Overall representation of the HLW repository architecture



Longitudinal section of a HLW cell during operation and after closure

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Model accounts for mineral, sorbed and aqueous concentrations

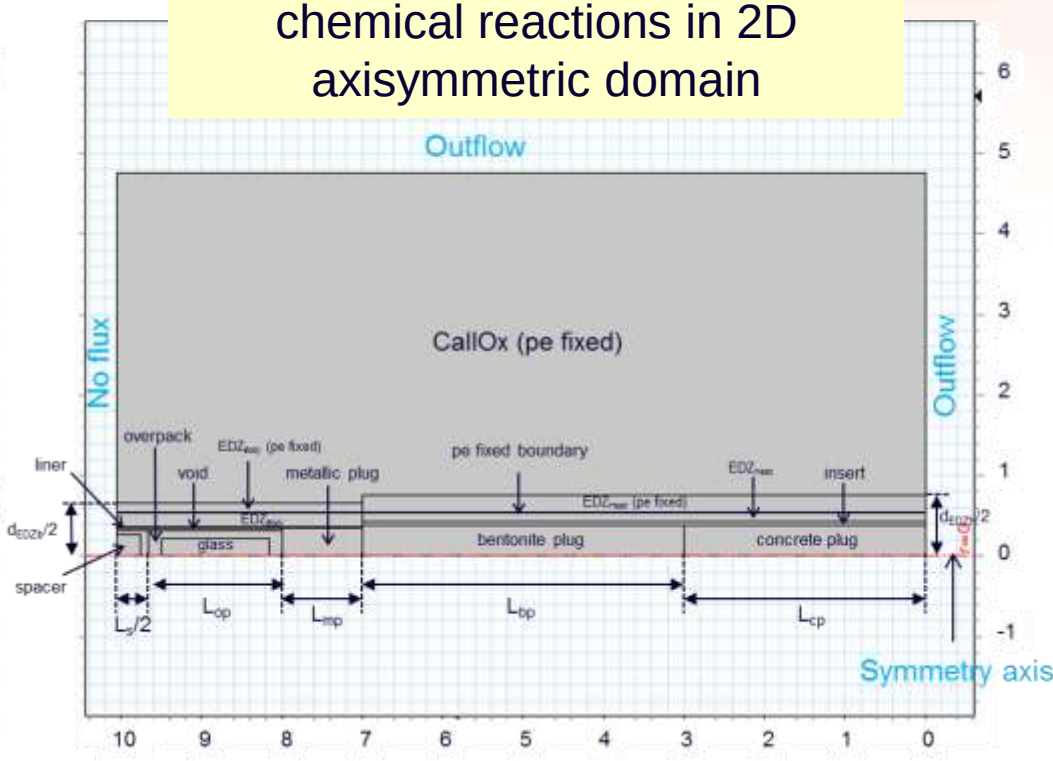
Geochemical system

A complex geochemical system foe each subdomain including radionuclides (Cs, Se, Tc, U), as well as sorption on and exchange within mineral phases

CallOx / CallOx EDZ	CallOx / CallOx EDZexchange	Steel Overpack, Liner, metallic plug	Concrete Plug
Illite		Steel dissolution rate	CSH1.6
Smectite		Magnetite	Ettringite
Chlorite	NaCox	Siderite	Calcite
Microcline	KCOx	H2(g)	CSH0.8
Pyrite	$CaCox_2$	Calcite	Etringite-Fe
Quartz	$MgCox_2$	Greenalite	Lizardite
Calcite	$FeCox_2$	Crondstedtite	SiO_2(am)
Dolomite	SrCox,	Berthierine	Magnetite
Siderite		Lizardite	Greenalite
Bentonite Plug		Vermiculite	Crondstedtite
Montmorillonite			Berthierine
Quartz			
Albite			
Microcline	**Bentonite plug exchange**		
Pyrite	NaX		
SiO_2(am)	KX		
Calcite	CaX_2		
Siderite	MgX_2		
Magnetite			
Greenalite	**Bentonite plug surface reactions**		
Crondstedtite	SsOH		
Berthierine	Sw_1OH		
Vermiculite	Sw_2OH		

Glass	Void
Glass dissolution rate	Calcite
SiO_2(am)	Siderite
Vermiculite	Magnetite
Calcite	Lizardite
Saponite	Vermiculite
Borax	Greenalite
Magnetite	Crondstedtite
Siderite	Berthierine
Greenalite	
Crondstedtite	
Berthierine	

Transport by diffusion and chemical reactions in 2D axisymmetric domain



Simulations with iCP

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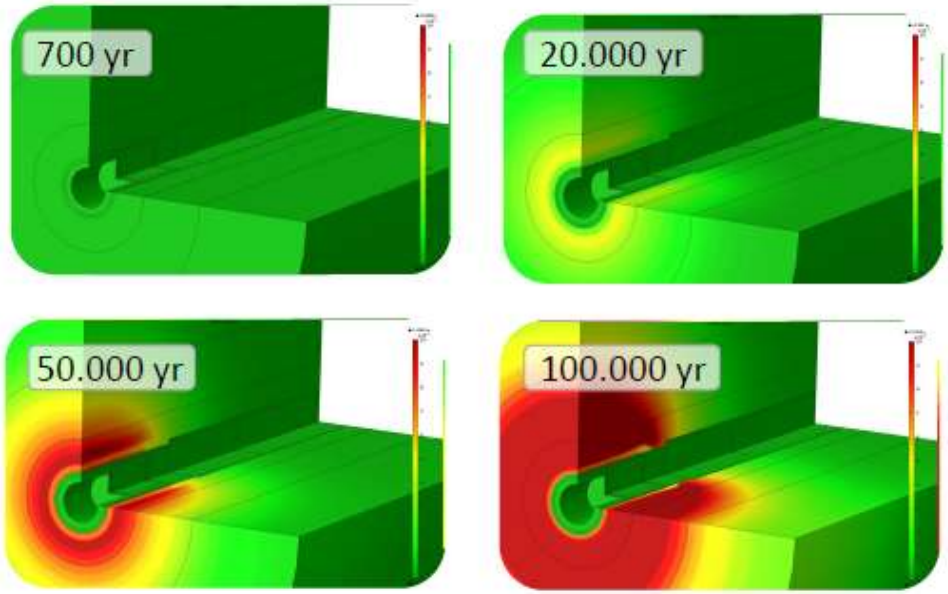
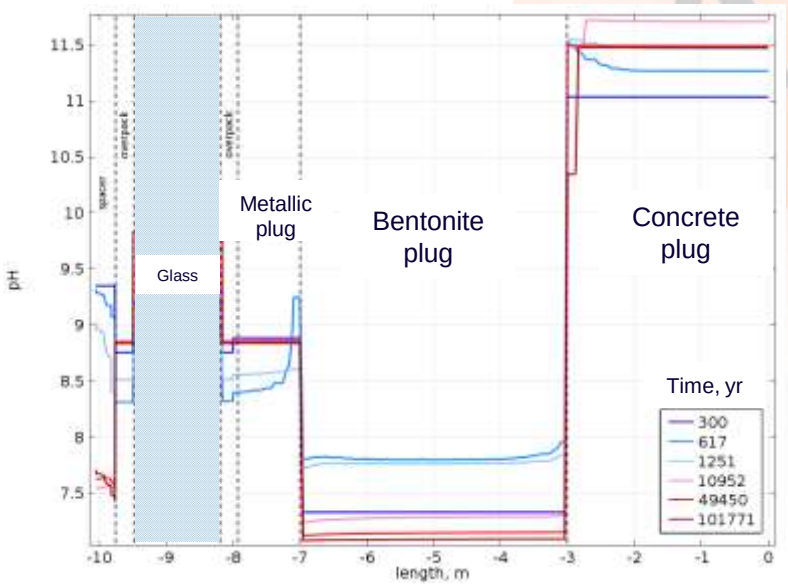
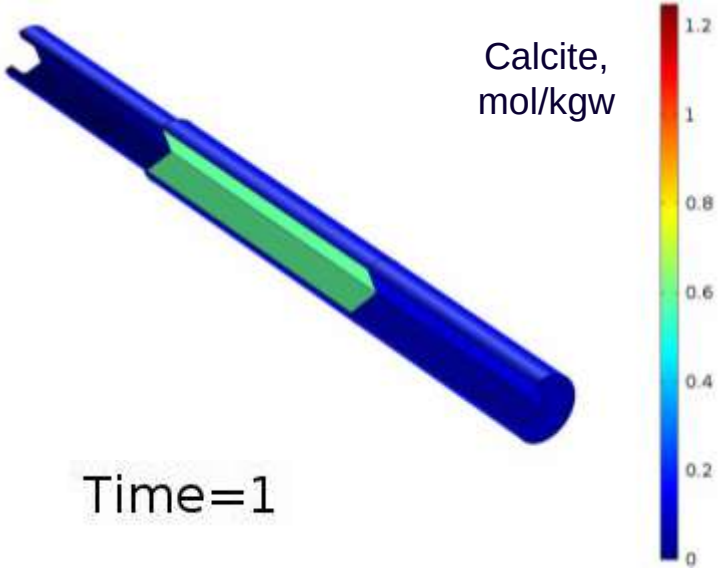
Radionuclide and mineral evolution





Retention of Cs as function of time within CallOx exchange positions



Summary

- Different modeling and simulation codes. Interfacing provides powerful tools (e.g., iDP, iCP) → **iMaGe platform**
- Important contribution to the development and assessment of different engineering solutions for nuclear waste disposal in SFR.
- Model of groundwater flow and transport can be used to optimize the design of the barriers from a hydrogeological perspective.
- Long-term simulations (up to 100,000 years) of flow and reactive transport at different scales have been performed successfully.

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- Peter Lichtner, OFM Research (USA)

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