AREHS: Effects of changing boundary conditions on the evolution of hydrogeological systems: Numerical long-term modeling considering thermal-hydraulic-mechanical (-chemical) coupled effects

Funded by: Bundesamt für die Sicherheit der nuklearen Entsorgung (BASE, Ref-ID: 4719F10402)

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safeND, Berlin, 13. - 15.09.2023

Objectives of AREHS

- **Understanding:** Increase the understanding of the impact of future warm and cold periods including glaciation on the geological system in the vicinity of the host rock

- **Concept:** Development of a consistent concept for quantification of the changes over a period of 1 mill yrs. as a basis for long term safety analysis

- **Workflow:** Development and verification of a THM(C) - modeling toolbox for all three types of host rocks (salt, clay and crystalline rocks)

Processes and numerical codes

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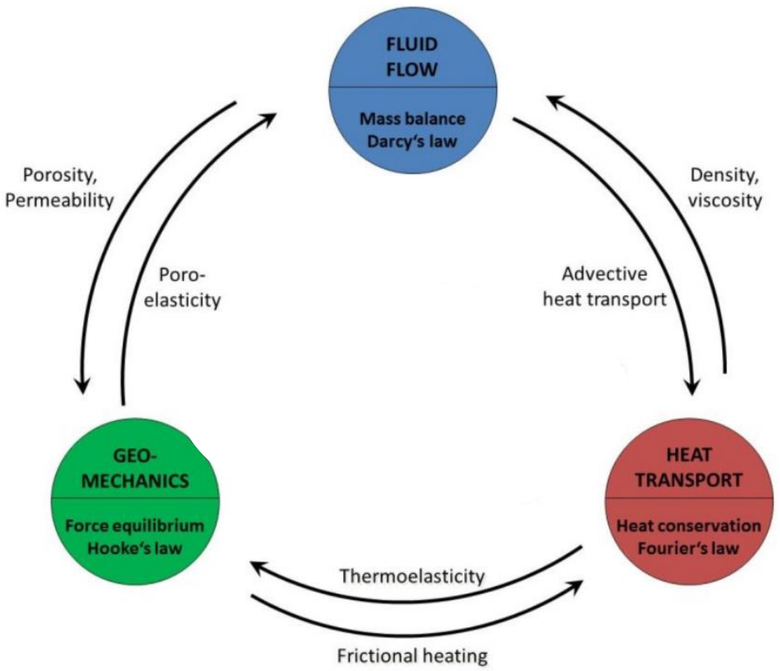
Basic processes and coupling based on FEP-tables:



From Gaucher u. a., 2015

Considering the spatial scale and the temporal scale of up to 1 mill yr

Numerical codes:

Salt rock:	OpenGeoSys
Clay rock:	OpenGeoSys
Crystalline rock:	3DEC + DFN.lab

Have been successfully verified

Workflow

OGS - Workflow Clay Rock and Salt Rock

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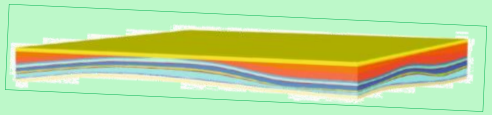
„manual“ input / automatically generated by transformations

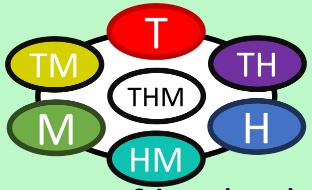
Transformation = automated routine

snakemake manages the transformations

Material parameters / models (csv)

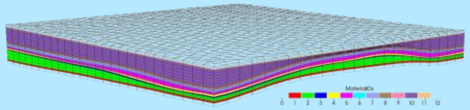


Surface meshes (GoCAD)

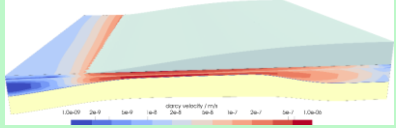


Project files (prj)

OGS model (prj)



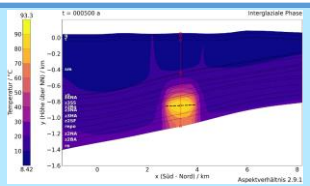
FEM – capable mesh (vtu)



Boundary conditions / Source terms (py)

OpenGeoSys

Simulation (pvd,xdmf)



Results (pdf)

Workflow Chrystalline Rock: 3DEC + DFN.lab

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→ *Development of a "DFN-DEM"* modelling workflow*

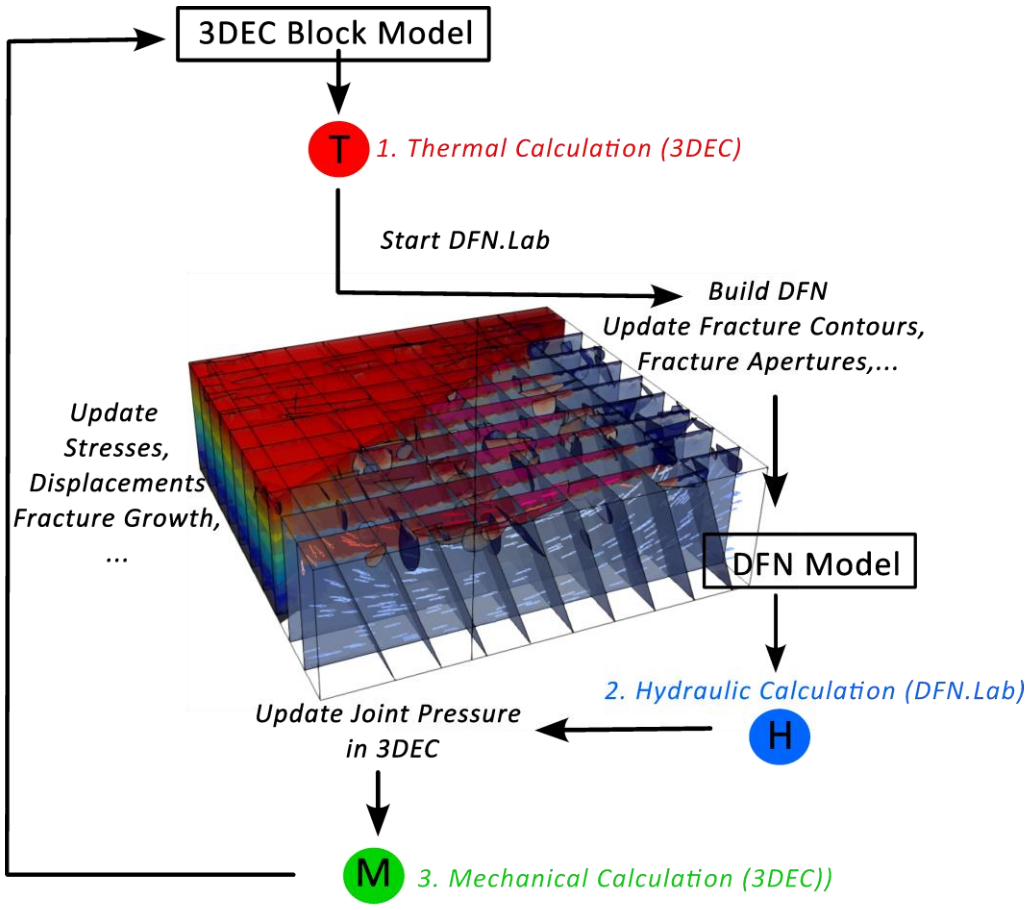
Combining the DEM-Software **„3DEC"** and DFN-Software **„DFN.Lab"**

→ **Idea: "outsourcing" flow calculation**

- 3DEC: thermal + mechanical calculation
- DFN.Lab: hydraulic calculation

→ **Realization:**

- Sequential THM calculation scheme
- 3DEC structure elements („subcontacts") used for "information exchange"
- Fracture contours, normal displacement/apertures, fluid pressure are constantly exchanged between 3DEC and DFN.Lab



**DEM = Distinct Element Method, 3DEC*
DFN = Discrete Fracture Network, DFN.Lab

Boundary Conditions and Geological Models

Driving boundary conditions

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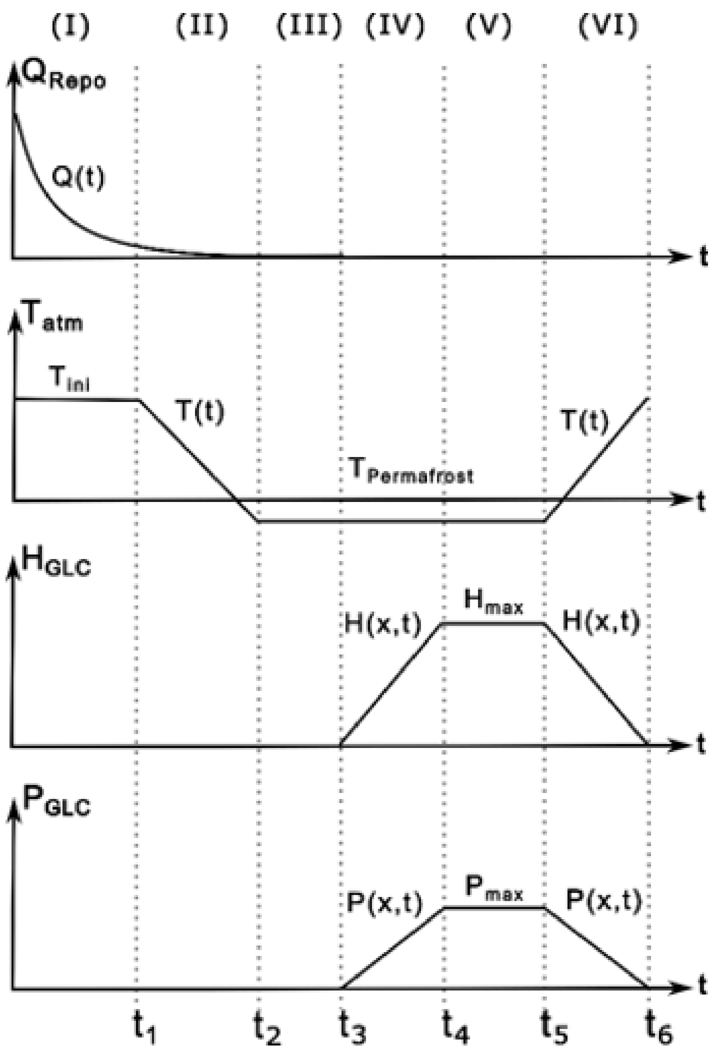
One cycle of warm and cold periods

Impact		Start	End	BC
Repository	Heat source	*0*	*5.000 years*	Q
Permafrost	Temperature Reduction	*5.000 years*	*15.000 years*	T
	Permafrost Temperature	*15.000 years*	*35.000 years*	T
Ice-Shield	Advance	*35.000 years*	*55.000 years*	THM
	Stagnation	*55.000 years*	*85.000 years*	THM
	Retreat	*85.000 years*	*95.000 years*	THM



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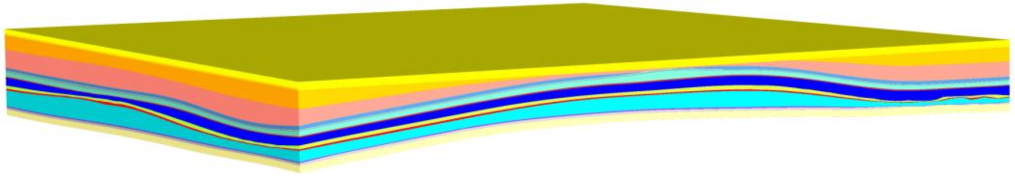
Geologcial models salt and clay based on the generic ANSICHT - models

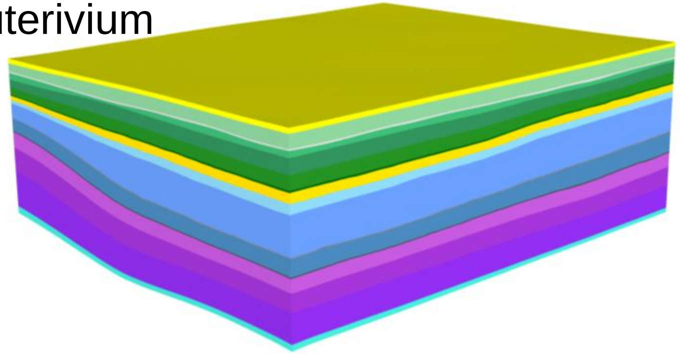
3D-Model: Salt (pillow)

Model area: 12 x 12 km², elevation: 85 m NN to -1400 m NN, Host rock: Staßfurt salt



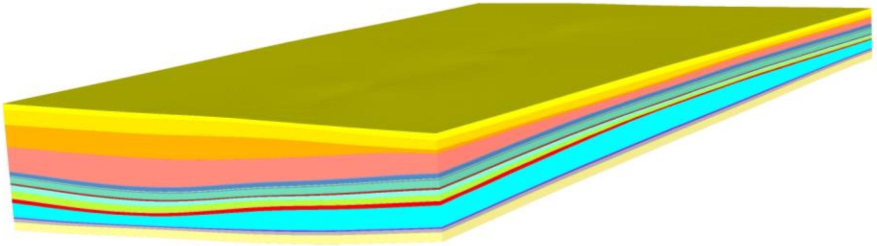
3D-Model: Clay (North Germany)

Model area: 12 x 10 km², elevation 130 m NN to -4200 m NN, Host rock: Barremium and Hauterivium



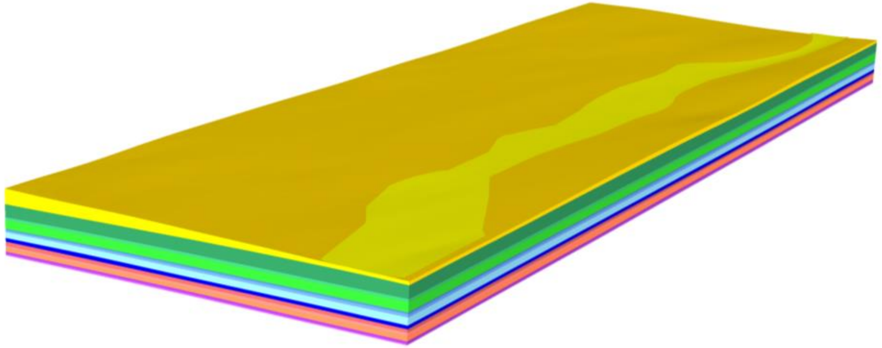
3D-Model: Salt (flat layering)

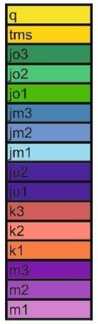
Model area: 10 x 7 km², elevation: 87 m NN to -1500 m NN, Host rock: Staßfurt salt



3D-Model: Clay (South Germany)

Model area: 22 x 7 km², elevation: 565 m NN to -666 m NN, Host rock: Opalinuston





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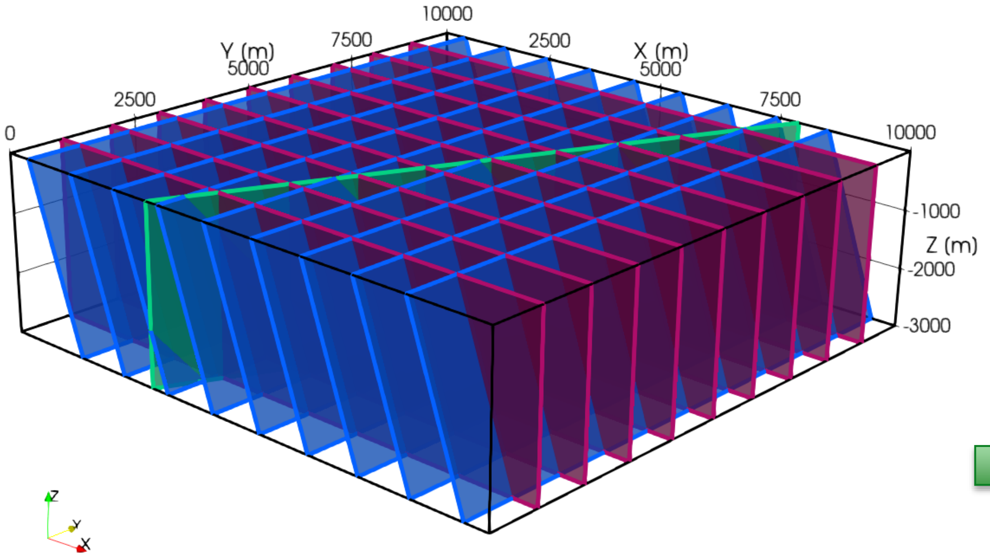
Synthetic geological model crystalline

3D-Model: Crystalline rock – multiple host rock (generic!)

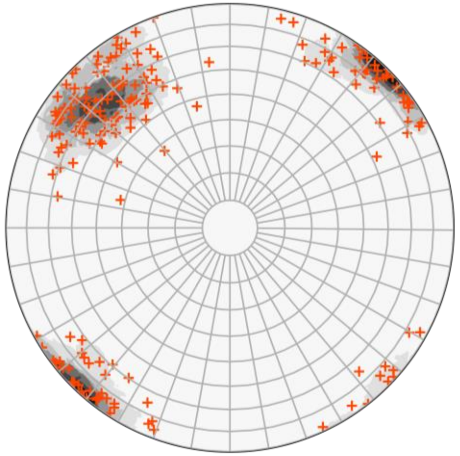
Deterministic Fault network

- Orthogonal fault network with 1 km distance
- NW-SE striking faults with 70° dips towards NE
- SW-NE striking faults with 90° dips and
- One NNW-SSE striking fault, vertical

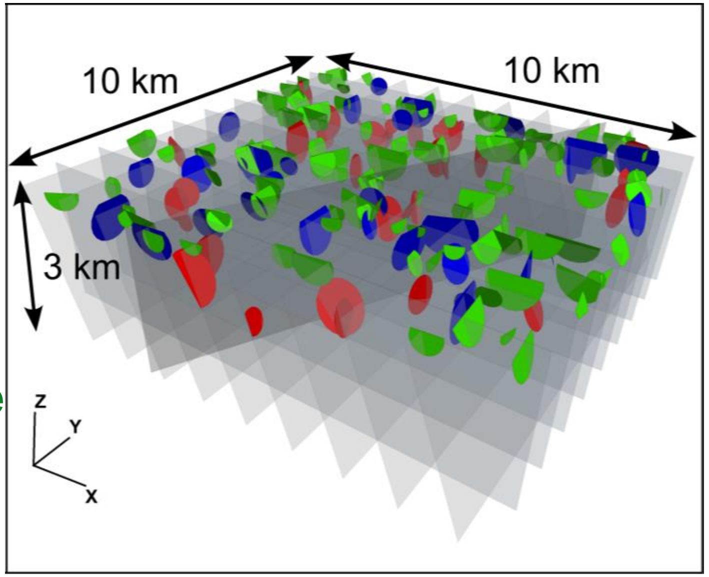


Stochastic DFN

- 2 Joint Sets,
- Fisher-Orientation,
- Power Law Fracture Length distribution (min: 300 m, max: 1000 m),
- Fracture density decreases with depth
- „hydraulic active" fractures (=isolated fractures are removed from DFN)



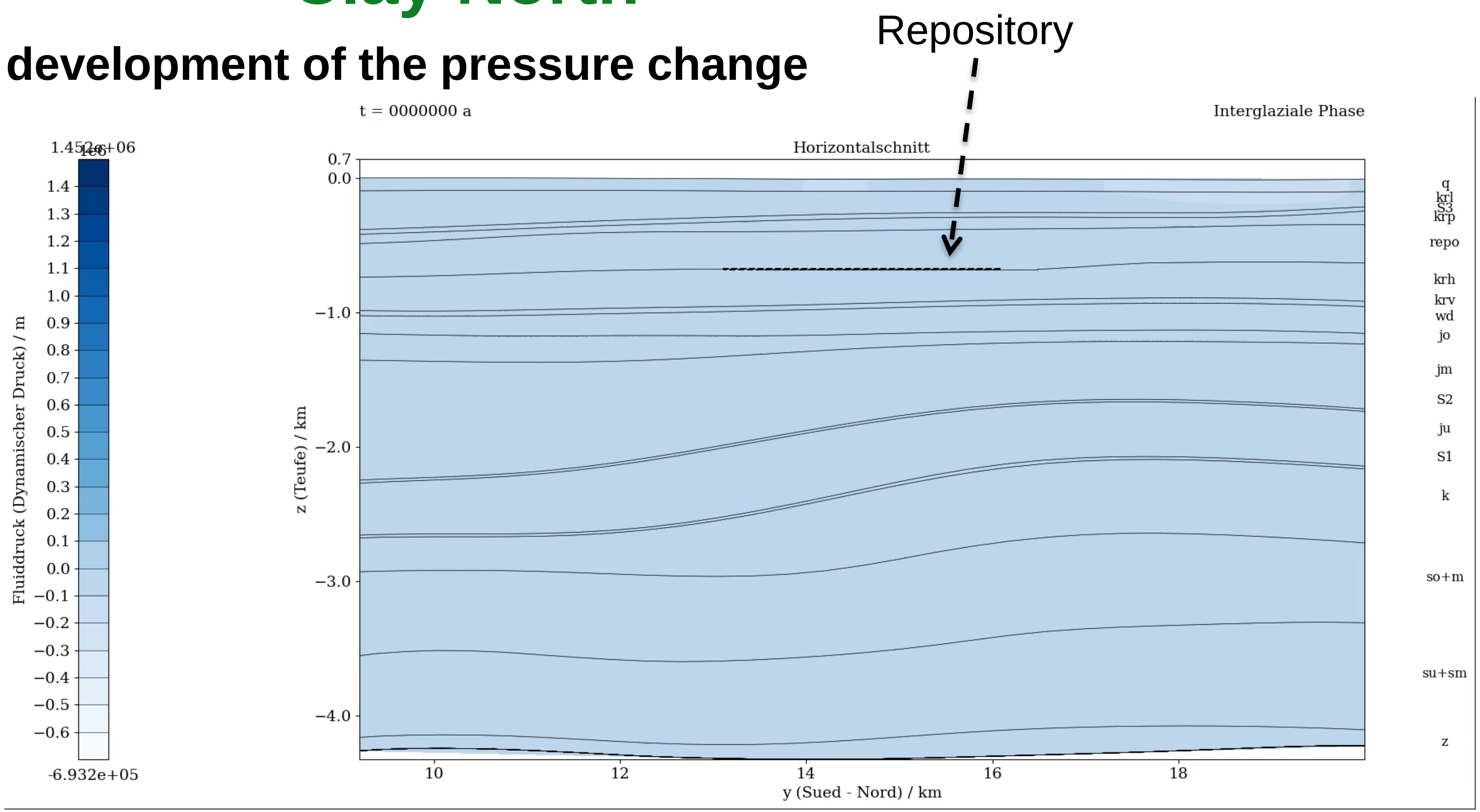
Fault and fracture network used as geological model for the numerical simulation „multiple host rock"



Selected results of the modeling of future glacial cycles on THM-(C) processes

Clay rock: Full glacial cycle model
Clay North

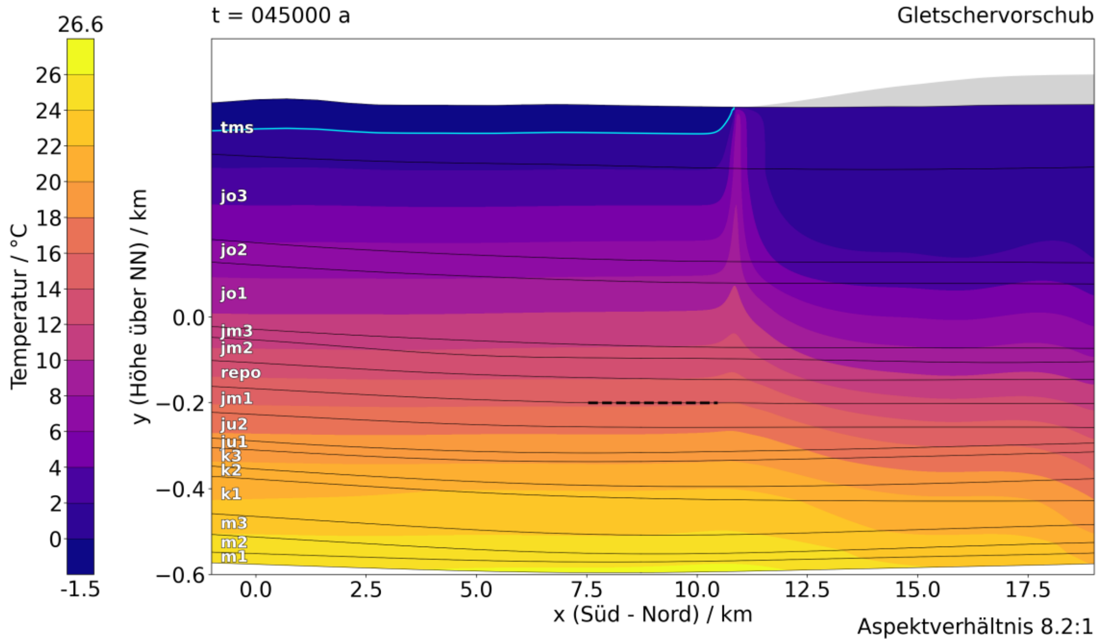
Temporal development of the pressure change



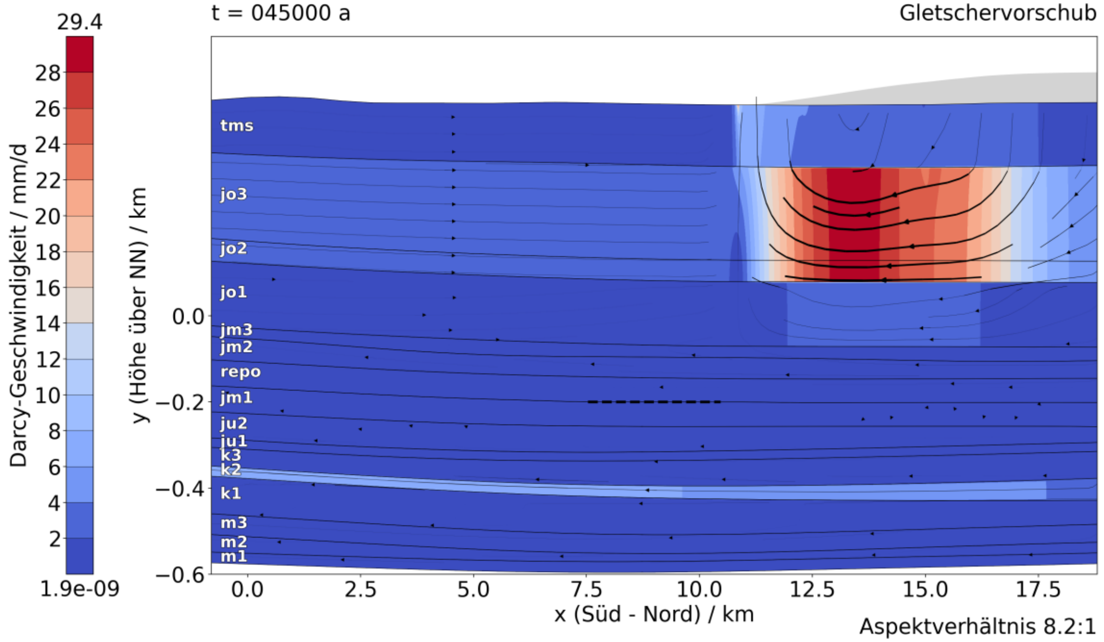
→ long-term (persistent) pressure anomalies due to THM coupling

Model Clay South: Temperature and Darcy velocity @45000 yr

Temperature



Darcy velocity



Convection induced by glacier BC and no flow BC caused by permafrost

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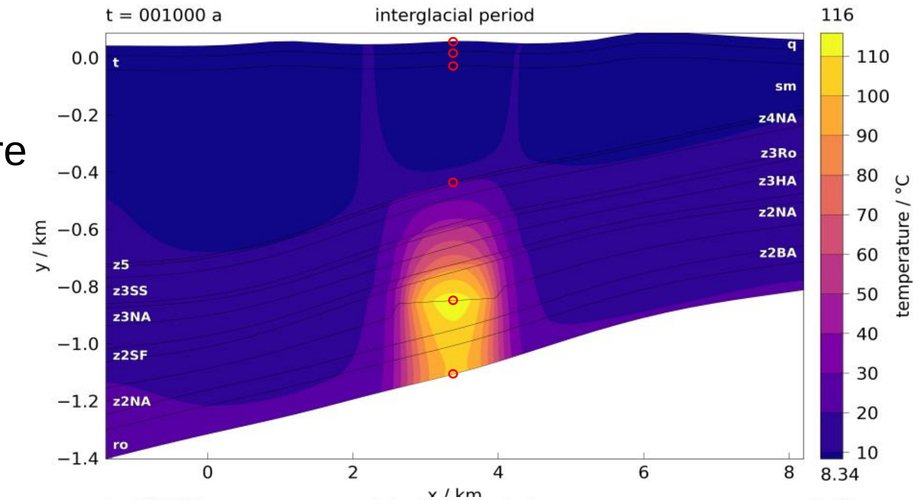
Salt rock: Two glacial cycles - Salt flat layering

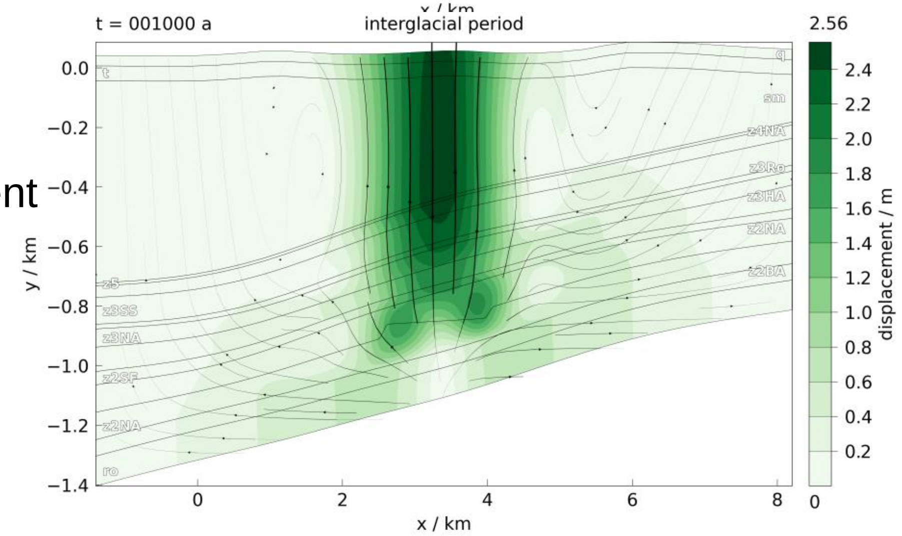
- Increasing temperature driven by repository heat
- Temperature driven displacement
- “Quick” dissipation of surplus heat
- No remaining influence in second cycle

1000 yr: repository heat prod

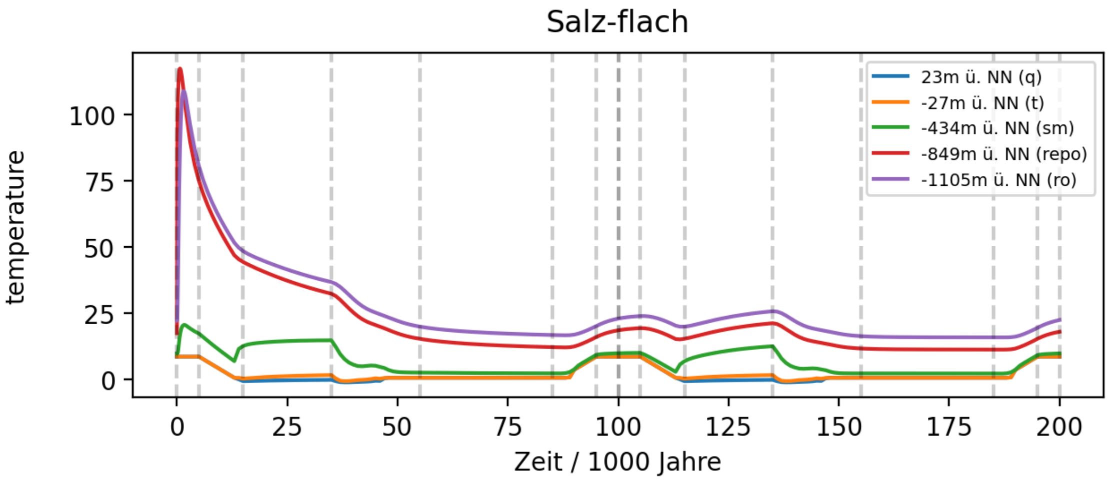
Temperature



Displacement



Temperature for different depths for two glacial cycles



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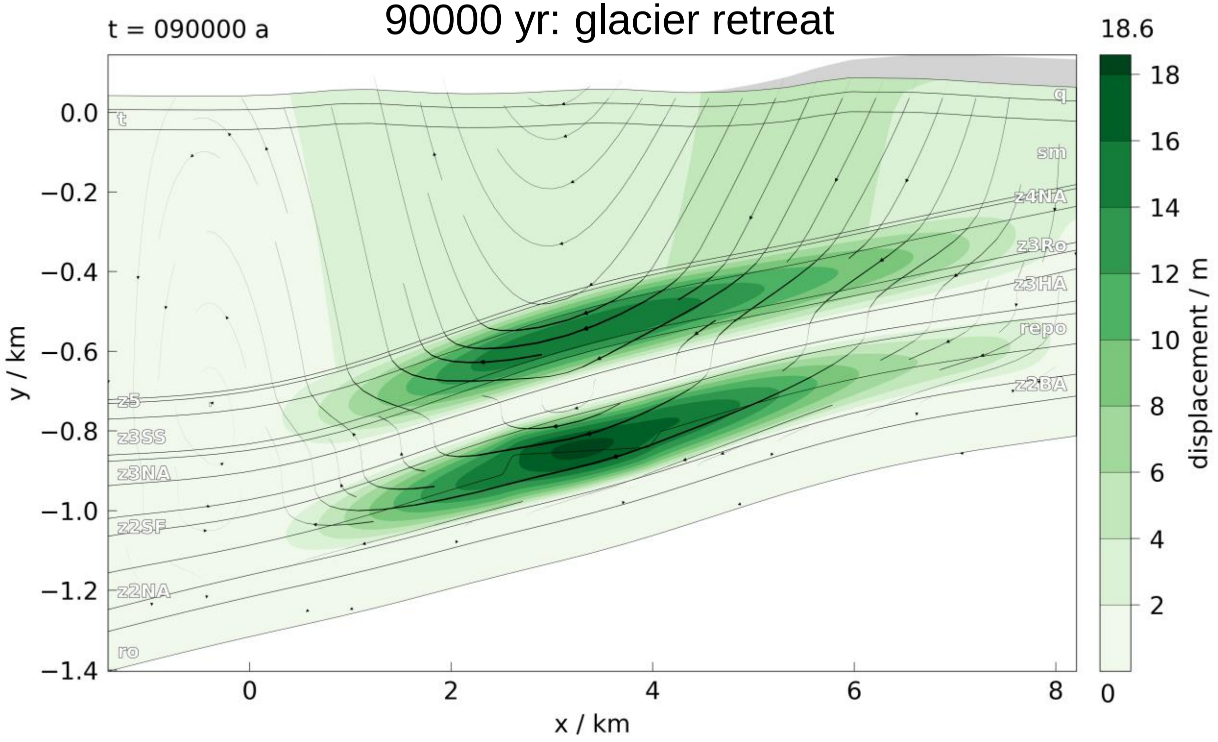
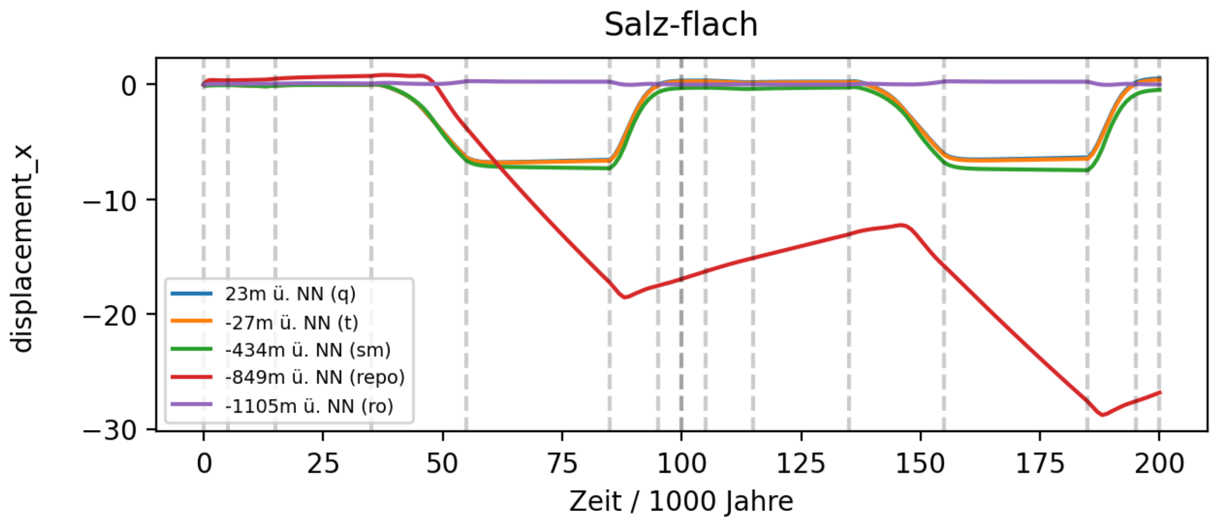
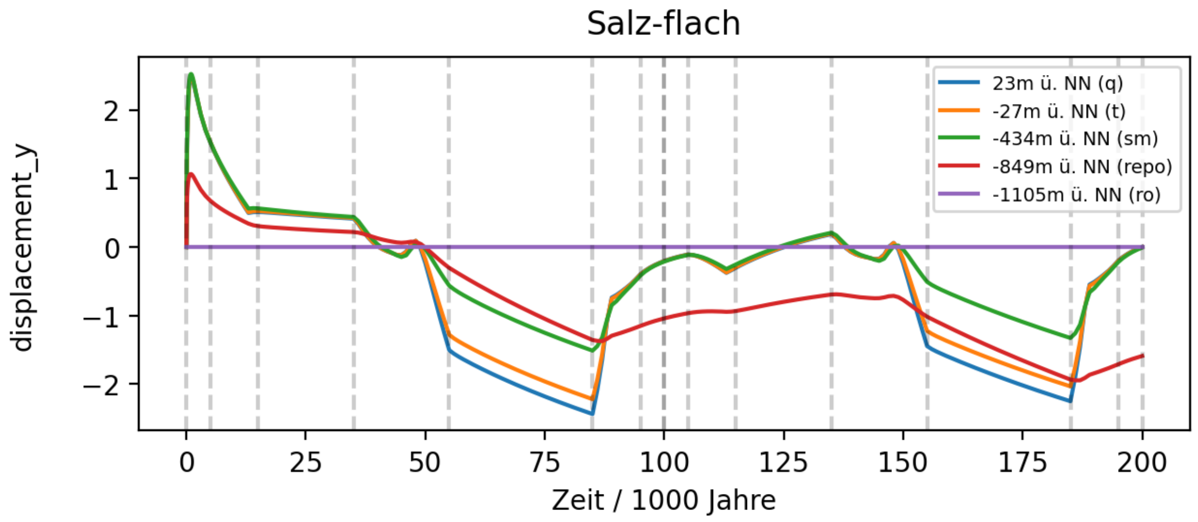
Salt rock: Two glacial cycles model salt flat layering

- Creep displacement accumulates in salt over time

90000 yr: glacier retreat







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Crystalline rock: Repository heating

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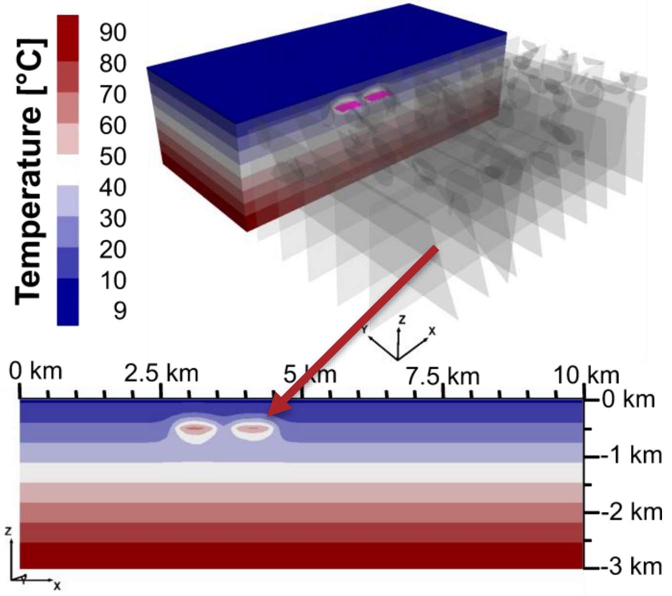
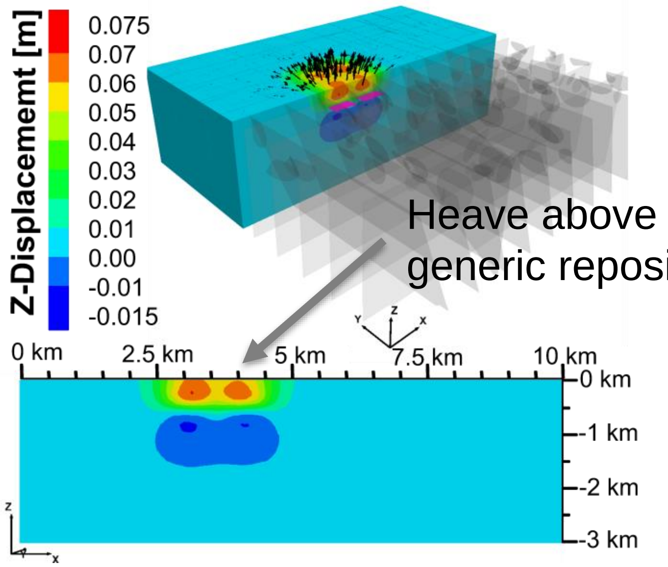
500 yr: repository heat prod

Generic Repository (=Heat Source)

- Located in (mainly) undisturbed model area





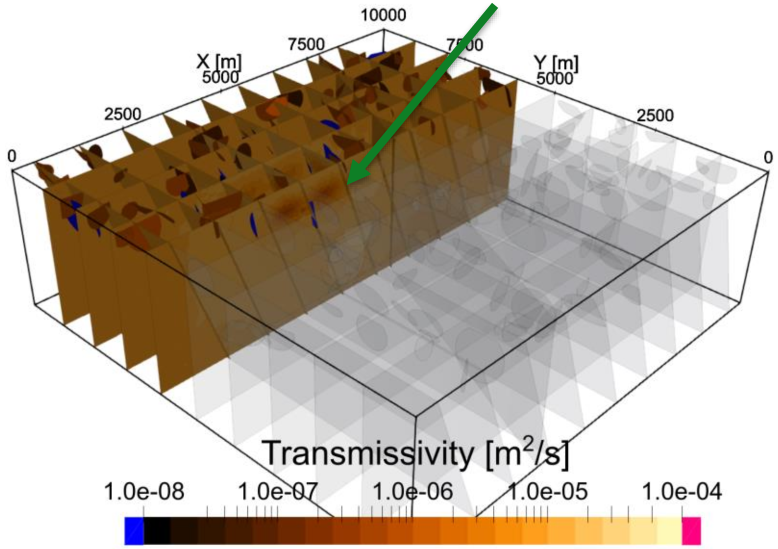
Heave above the generic repository

Thermal Stresses:

→ Increase of horizontal compression at repository level

→ Decrease of horizontal compression at model surface

Fault Closure in the vicinity of the generic repository



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Crystalline rock: Selected simulation results: Periglacial and glacial conditions

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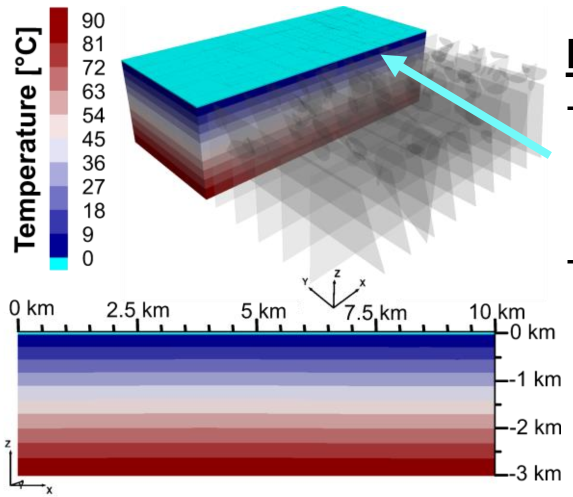
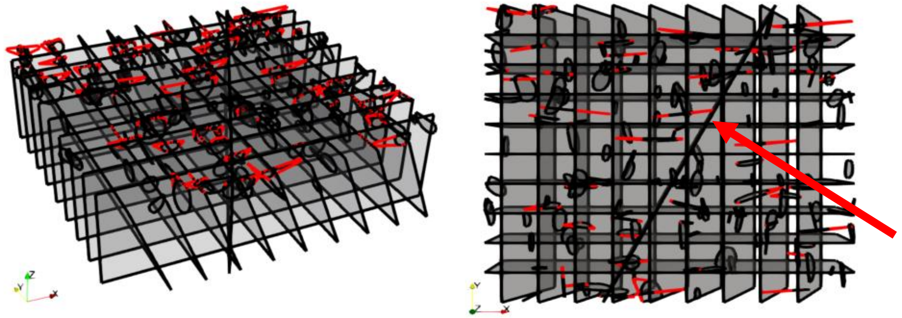


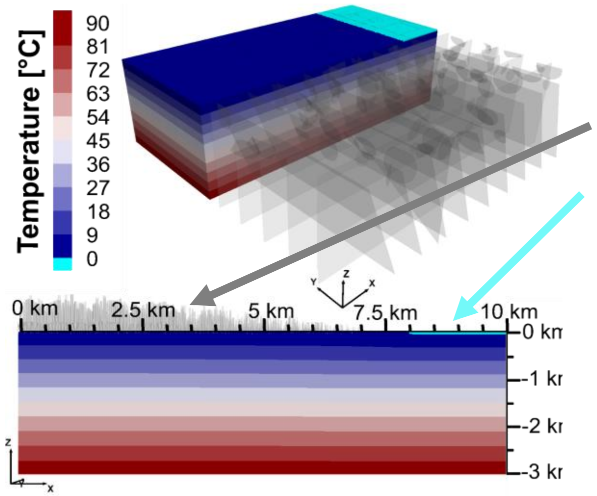
Periglacial Conditions

- Formation of a continuos permafrost layer
- ~50 m depth



35000 yr: periglacial conditions

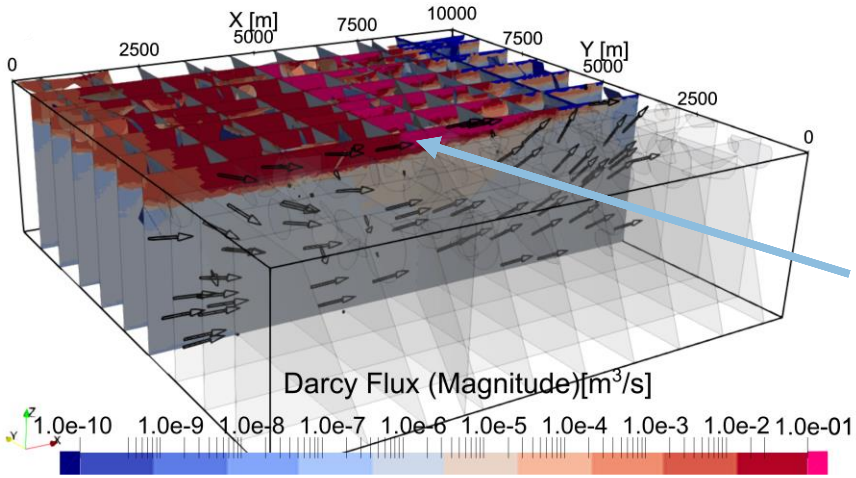
Thermal contraction triggers fracture growth (particularly close to model surface)



Glacial Conditions

Ice-sheet

proglacial permafrost



80000 yr: glacial conditions

Concentrated fluid infiltration beneath ice-shield

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Summary and future research

Summary

Clay rock

- Glacial cycles lead to persistent fingerprints of THM events
- Results depend on mechanical material model

Salt rock

- Permanent changes in displacement field due to viscoplastic creeping
- Creep at small deviator stresses contributes to efficient removal of deviator stresses.

Chrystalline rock

- “Self sealing” of the repository in the heating phase due to increased stresses
- Permafrost leads to rock failure and increase of transmissivity at surface
- Intensive water infiltration beneath the glacier leading to preverential flow pattern and possible reactivation of faults.
- **Simulaton „covered repository“ scenario by extraction of the BC from clay model**

Summary

General summary

- The simulation results correspond to trends reported in literature very well
- Full THM-process coupling is essential because all couplings show effects on the results
- The flow field in the underground completely changes in a warm – cold cycle
- Workflow as a solid basis to investigate specific sites in more detail
- Strong influence of BCs (effects of domain size have to be considered) → Mechanical BCs could also be extracted from larger-scale simulations
- Results could be used as boundary conditions for models on smaller scales, e.g. for detailed repository models

Future research (selected items)

- Alternative material models need further investigation
- The whole OGS – workflow is ready for HPC and has successfully tested but needs further optimization
- Incorporation of far field effects has to be investigated
- Fault zones only have been explicitly investigated in crystalline rock, not in clay and salt rock
- The initial thermal, hydraulic and stress conditions have been simplified, they are much more complex for real sites

AREHS:
Effects of changing boundary conditions on the evolution of hydrogeological systems: Numerical long-term modeling considering thermal-hydraulic-mechanical (-chemical) coupled effects (Ref-ID: 4719F10402)

Disclaimer: The presentation reflects the opinion of the AREHS research team but does not necessarily represent the opinion of BASE

Thank you for your attention on behalf of the

AREHS team!

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