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Numerische Verfahren zur Quantifizierung der Auswirkung von Parameterungewissheiten auf die Ergebnisse THM-gekoppelter Integritätsberechnungen – MeQUR

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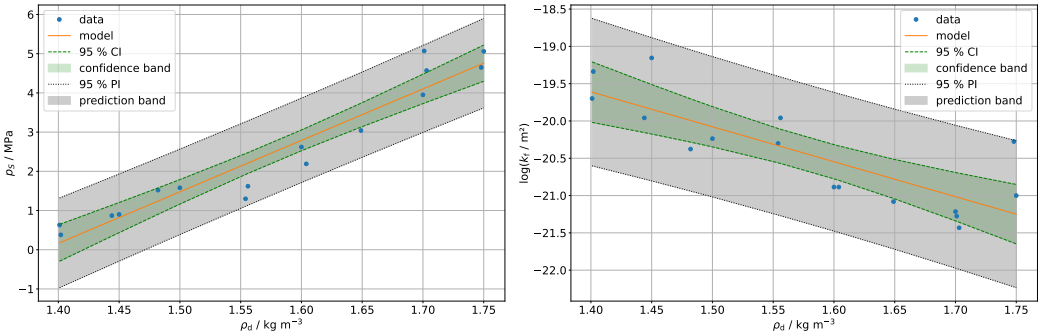
[3] Helmholtz-Zentrum für Umweltforschung GmbH – UFZ
[4] Bundesanstalt für Geowissenschaften und Rohstoffe (BGR)

06.02.2025

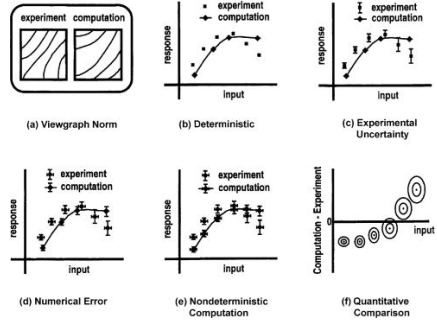
Statistical uncertainty of material parameters

Dry-density dependent maximum swelling pressure and intrinsic permeability of bentonite:



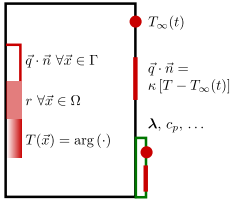
UQ – how can it enrich the picture?

- Transfer information on “imprecision” to numerical safety investigations
- Aid model choices (process models, constitutive models, correlations/transformation models)
- Demonstrate existence of potential gaps in models
- Provide natural context for V&V (what can we aim for)
- Link to parameter identification
- Overall context for relative relevance assessment (ranking) of features

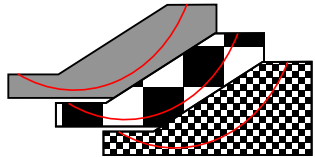


From [OTH04].

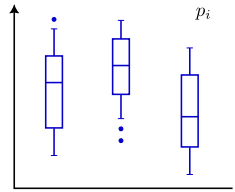
Sources of uncertainty



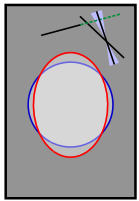
bc representation



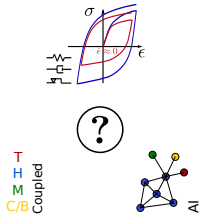
heterogeneity / scale ratios / variance reduction



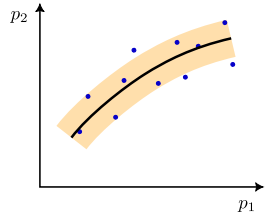
parameters



geometry, connectivity



conceptual modelling choices

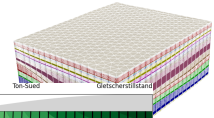


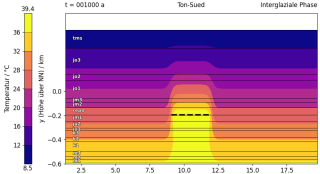
transformation

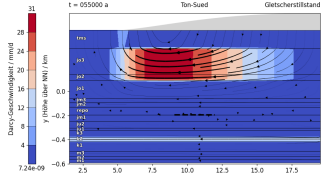
Ziele

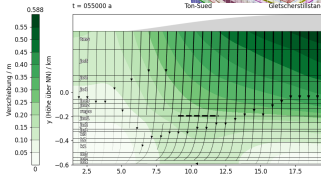
- **Methodenentwicklung** für UQ und SA für THM-gekoppelte numerische Integritätsanalysen der geologischen Barriere im Rahmen von Sicherheitsuntersuchungen
- Verbindung von **mathematischer Konsistenz und Praxistauglichkeit** der Methoden
- **Prüfung & Demonstration** des Konzepts anhand zweier Fallstudien, die unterschiedliche räumliche und zeitliche Skalen adressieren
- **Visualisierung** ungewissheitenbehafteter Simulationsergebnisse
- **Rückschlüsse** auf verbesserte Untersuchungsprogramme ableiten und sicherheitstechnische Bewertung der Ergebnisse zu unterstützen

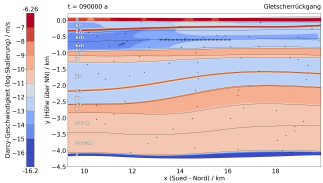
Far-field

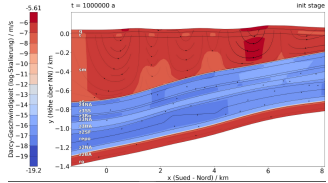


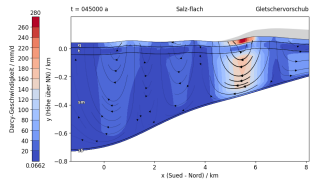

t = 001000 a
Ton-Sued
Interglaziale Phase
Temperatur / °C
y (Höhe über NN) / km
x (Sued - Nord) / km


t = 055000 a
Ton-Sued
Gletscherstillstand
Darcy-Geschwindigkeit / mm/d
y (Höhe über NN) / km
x (Sued - Nord) / km

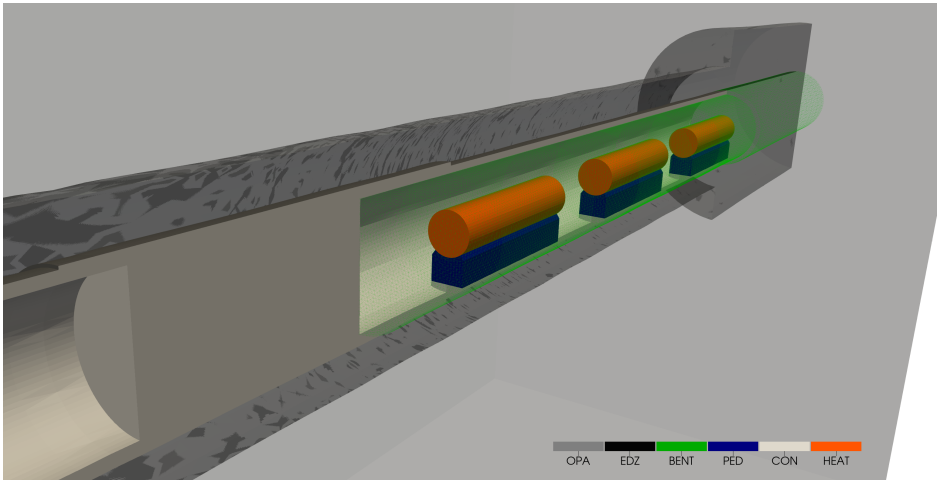

t = 055000 a
Ton-Sued
Gletscherstillstand
Verschiebung / m
y (Höhe über NN) / km
x (Sued - Nord) / km


t = 090000 a
Gletscherrückgang
Darcy-Geschwindigkeit (log Skalierung) / m/s
y (Höhe über NN) / km
x (Sued - Nord) / km


t = 1000000 a
init stage
Darcy-Geschwindigkeit (log Skalierung) / m/s
y (Höhe über NN) / km
x (Sued - Nord) / km

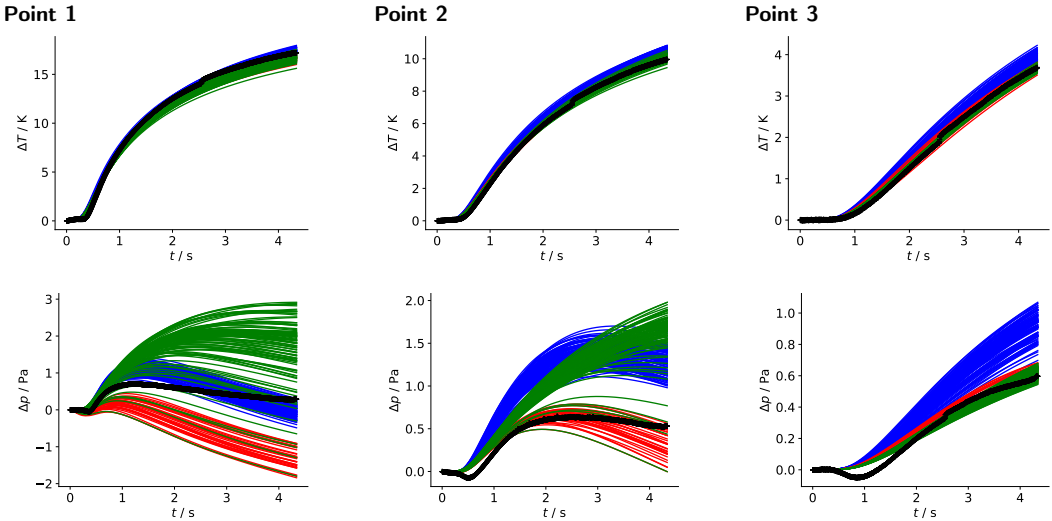

t = 045000 a
Salz-flach
Gletschervorschub
Darcy-Geschwindigkeit / mm/d
y (Höhe über NN) / km
x (Sued - Nord) / km

Near-field



From [Kai+25]

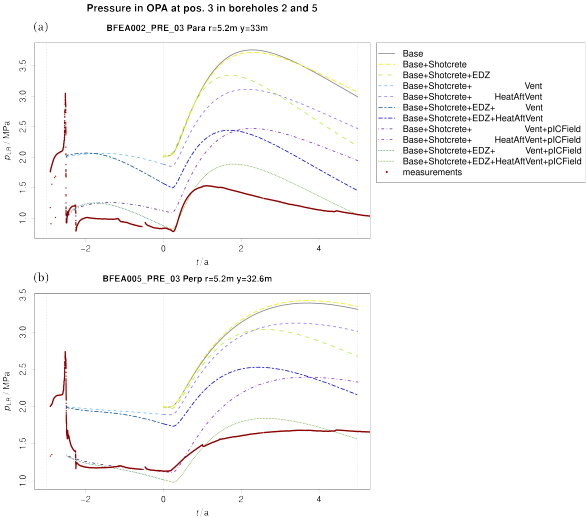
Comparison to in situ measurements – parameter uncertainty



History match subsampling to point 1/2/3.

[RKN24].

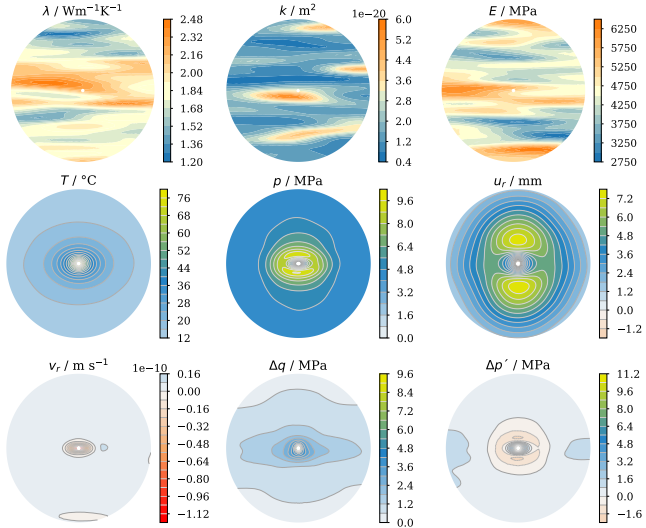
Comparison to in situ measurements – model complexity



- Sensor location uncertainty
- Excavation
- Ventilation
- Shotcrete
- Contouring
- Backfill
- EDZ
- Constitutive model
- ...

[Kai+25]

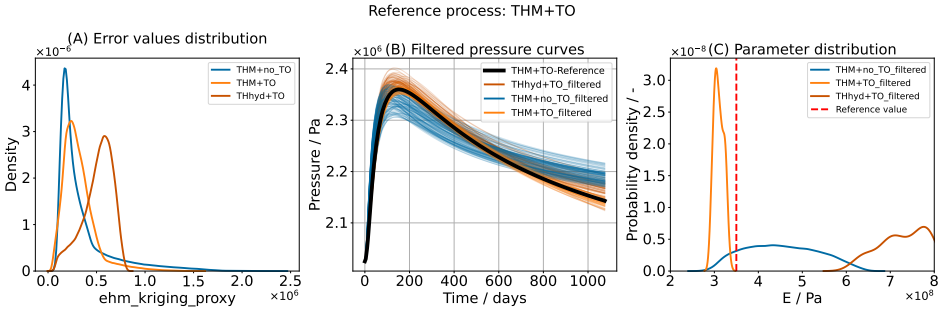
Spatial variability – from random variables to random fields



[Cha+25]

Process model selection

- Addition of thermo-osmosis adds additional (free) parameters?
- Can thermal pore pressurization be better reproduced with more complex physics?
- Can we obtain information about suitable process models from UQ analyses and use them for parameter identification?



[Nag+24]

Output

"...the Bear People are here..."

Output so far...

Software:

- OGSTools for GSA, Sampling workflows, surrogate modelling around OGS
- Kleme: Random fields, linked to OGS
- Julia library for UQ and SA based on distributed sparse grids
- Online tool for interactive exploration of parameter space

Publications:

- 8 journal articles + 2 in preparation
- 15+ conference contributions
- 5 invited talks
- 1 MSc thesis finished, 2 PhD theses soon to be finished

Weiterer Ablauf

Vortrag:

1. Quellen von Ungewissheiten – Von Daten zu Modellen (Sibylle Mayr, Oliver Ernst)
2. Die Anwendung: Probabilistische Integritätsanalysen der geologischen Barriere (Max Bittens)

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3. Probabilistische Analyse von URL Versuchen (Jörg Buchwald)
4. Räumliche Variabilität (Aqeel Chaudhry)
5. Modellselektion (Feliks Kiszkurno)

Posters:

1. Feliks Kiszkurno: Is more always better? Study on uncertainties introduced by decision-making process of model design and thermo-osmosis
2. Aqeel A. Chaudhry: Effects of Inhomogeneity and (Statistical and Material) Anisotropy on THM Simulations
3. Jobst Maßmann: Statistical analyses on the relevance of thermal data for the safety-related assessment of repository systems – some results from the project ThermoBase
4. Sibylle Mayr: Physical origins of the uncertainties of the predominant input parameters
5. Maximilian Bittens: Probabilistic integrity analyses for a generic high-level radioactive waste repository

Danksagung

BGE BUNDESGESELLSCHAFT FÜR ENDLAGERUNG

MeQUR wird im Rahmen des URS Verbundprojekts durch die Bundesgesellschaft für Endlagerung (BGE) finanziert und unterstützt.

Wir danken der BGE und dem gesamten OGS Entwicklungsteam für die Unterstützung.

AP Struktur I

Bereitstellung konsistenter Eingangsdaten

AP1 Analyse physikalischer Ursprünge von Parameterunsicherheiten, statistische Aufarbeitung der experimentellen Datenbasis

*(**BGR**; TUChem, TUBAF)*

Mathematische Methoden und Algorithmen

AP2 Anpassung, Entwicklung und Demonstration ausgewählter mathematischer Methoden der Quantifizierung von Ungewissheiten und Sensitivitäten für gekoppelte THM Analysen

*(**TUChem**; TUBAF, UFZ, BGR)*

AP3 Integration numerischer Prozessmodelle mit UQ Analysemethoden unter Berücksichtigung von Methoden des Hochleistungsrechnens

*(**UFZ**; TUBAF, TUChem, BGR)*

AP Struktur II

Anwendung der UQ- und SA-Methoden in verschiedenskaligen Fallstudien

AP4 Szenariensimulationen zu unscharfen THM-Analysen von URL-Versuchen

*(**TUBAF**; BGR)*

AP5 Szenariensimulationen zu unscharfen THM-Analysen für Integritätsnachweise am generischen Endlagersystem ohne direkten Standortbezug

*(**BGR**; TUBAF)*

AP6 Globale Sensitivitätsanalysen zur Ermittlung der die Zielgrößenungewissheiten dominierenden Eingangsparameter

*(**BGR**; TUBAF, TUChem)*

AP Struktur III

Ergebnisinterpretation und -verwertung.

AP7 Untersuchung der „messtechnischen Präzisierbarkeit“ der dominanten Eingangsparameter
*(**BGR**)*

AP8 Darstellung von Ungewissheiten in Integritätsnachweisen unter Nutzung integrierter 3D-Visualisierungsmodelle
*(**UFZ**)*

AP9 Ableitung von Handlungsempfehlungen für die Analyse im Kontext von vSU
*(**BGR**; TUBAF, TUChem, UFZ)*

Koordination

AP10 Projektkoordination und Ergebnistransfer
*(**TUBAF**; BGR, TUChem, UFZ)*

Output I

Software:

- OGSTools for GSA, Sampling workflows, surrogate modelling around OGS
- Kleme: Random fields, linked to OGS
- Julia library for UQ and SA based on distributed sparse grids
- Online tool for interactive exploration of parameter space

Journal articles:

[1] A.A. Chaudhry, C. Zhang, O.G. Ernst, **T. Nagel**.
Effects of inhomogeneity and statistical and material anisotropy on THM simulations.
Reliab Eng and Syst Safety, 110921, 2025.

[2] F. Kiszkurno, J. Buchwald, C.B. Silbermann, O. Kolditz, T. Nagel.
Is more always better? Study on uncertainties introduced by decision-making process of model design – a case study with thermo-osmosis.
In press.

Output II

[3] J. Buchwald, N. Grunwald, W. Wang, H. Shao, O. Kolditz, T. Nagel.
The relevance of two-phase flow in the thermo-hydro-mechanical evolution of clay formations exposed to high temperatures by heat-emitting waste.
Appl Therm Eng, 264, 125379, 2025.

[4] T. Nagel, J. Buchwald, F. Kiszkurno, M. Pitz, T. Helfer.
Hierarchical modelling in benchmarking, analysis and code development for coupled geo-processes.
Proc Appl Math & Mech, e202400025, 2024.

[5] M. Bittens.
OpenGeoSysUncertaintyQuantification.jl: a Julia library implementing an uncertainty quantification toolbox for OpenGeoSys.
J Open Source Softw, 9(98), 2024.

[6] K. Kurgyis, P. Achtziger-Zupančič, M. Bjorge, M.S. Boxberg, M. Broggi, J. Buchwald, O.G. Ernst, J. Flügge, A. Ganopolski, T. Graf, P. Kortenbruck, J. Kowalski, P. Kreye, P. Kukla, S. Mayr, S. Miro, T. Nagel, W. Nowak, S. Oladyshkin, A. Renz, J. Rienäcker-Burschil, K.J. Röhlig, O. Sträter, J. Thiedau, F. Wagner, F. Wellmann, M. Wengler, J. Wolf, W. Rühaak.
Uncertainties and robustness with regard to the safety of a repository for high-level radioactive waste: introduction of a research initiative.
Environ Earth Sci, 83(82), 2024.

Output III

[7] J. Buchwald, O. Kolditz and T. Nagel.
Design-of-Experiment (DoE) based history matching for probabilistic integrity analysis — a case study of the FE-experiment at Mont Terri.
Reliab Eng and Syst Safety, 244, 109903, 2024.

[8] M. Bittens, R.L. Gates.
DistributedSparseGrids.jl: A Julia library implementing an Adaptive Sparse Grid collocation method.
J Open Source Softw, 8(83), 2023.

Conference contributions:

[1] J. Buchwald, W. Wang, N. Grunwald, T. Nagel, O. Kolditz.
Hierarchical benchmarking of Richards-based thermo-hydro-mechanical coupled models for repositories of high-level radioactive waste.
In *9th Clay Conference*.
25–28 Nov, 2024, Hannover, Germany.

[2] M. Bittens, J. Thiedau, J. Maßmann.
Quantifizierung von Ungewissheiten in Integritätsanalysen der geologischen Barriere von Endlagersystemen.
In *Tage der Standortauswahl*.
18–19 April, 2024, Gosslar, Germany.

Output IV

[3] A.A. Chaudhry, C. Zhang, O. Ernst, T. Nagel.

Auswirkungen von Heterogenität und Anisotropie auf die Integrität der geologischen Barriere eines Endlagers für hochaktive Abfälle.

In *Tage der Standortauswahl*.

18–19 April, 2024, Gosslar, Germany.

[4] K. Kurgyis, J. Flügge, T. Graf, J. Kowalski, K.J. Röhlig, F. Wellmann, T. Nagel.

Einführung einer Forschungsinitiative über Ungewissheiten und Robustheit im Zusammenhang mit der Sicherheit von Endlagern für hochradioaktive Abfälle.

In *Tage der Standortauswahl*.

18–19 April, 2024, Gosslar, Germany.

[5] F. Kiszkurno, J. Buchwald, O. Kolditz, T. Nagel.

Hypothesis-testing and assisted-history-matching applied to evaluate uncertainty of model selection and parameter values: a case study of the impact of thermo-osmosis.

In *Geophysical Research Abstracts Vol. 26, EGU General Assembly*.

14–19 April, 2024, Vienna, Austria.

Output V

[6] T. Nagel, J. Buchwald, F. Kiszkurno, M. Pitz, T. Helfer et al.
Ungewissheiten und Modellkomplexität in vergleichenden THM Analysen: Zweiphasenfluss und Thermo-Osmose.
In *Trust in Models. Second workshop at the Federal Office for the Safety of Nuclear Waste Disposal.*
13–14 Mar, 2024, Berlin, Germany.

[7] M. Pitz, J. Thiedau, J. Maßmann, S. Kaiser, J. Buchwald, T. Nagel.
Calibration of Numerical THM Coupled Models to Experimental Data from the FE Experiment: Results and Experiences.
In *2nd International DECOVALEX Symposium on Coupled Processes in Radioactive Waste Disposal and Subsurface Engineering Applications.*
14–16 Nov, 2023, Troyes, France.

[8] T. Nagel, M. Bittens, J. Buchwald, A.A. Chaudhry, O.G. Ernst, W. Gräsle, F. Kiszkurno, K. Kurgyis, J. Maßmann, S. Mayr, J. Thiedau, C. Zhang.
Methods for the quantification of uncertainties in THM simulations for safety analyses.
In *Interdisciplinary Research Symposium on the Safety of Nuclear Disposal Practices safeND 2023.*
13–15 Sept, 2023, Berlin, Germany.

Output VI

[9] M. Bittens.
OgsUQ: an Uncertainty Quantification Toolbox for OpenGeoSys.
In *IAM Conference on Mathematical & Computational Issues in the Geosciences.*
19–22 June, 2023, Bergen, Norway.

[10] A.A. Chaudhry, D. Naumov, W. Wang, T. Nagel.
Coupled numerical modeling of the China Mock-Up experiment for swelling clay barriers.
In *15th Annual International Conference on Porous Media.*
22–25 May, 2023, Edinburgh, Scotland.

[11] J. Buchwald, S. Kaiser, W. Wang, O. Kolditz, T. Nagel.
DoE-based history matching for probabilistic integrity analysis – a case study of the FE-experiment at Mt. Terri.
In *15th Annual International Conference on Porous Media.*
22–25 May, 2023, Edinburgh, Scotland.

[12] F. Kiszkurno, J. Buchwald, O. Kolditz, T. Nagel.
Investigation on the impact of thermo-osmosis on fluid pressurisation in Boom clay – a case study of the ATLAS in-situ full-scale heating experiment.
In *15th Annual International Conference on Porous Media.*
22–25 May, 2023, Edinburgh, Scotland.

Output VII

[13] J. Buchwald, S. Kaiser, W. Wang, O. Kolditz, T. Nagel.
Uncertainty reduction by DoE-based history matching of the FE-experiment at Mt. Terri.
In *Geophysical Research Abstracts Vol. 25, EGU General Assembly*.
23–28 April, 2023, Vienna, Austria.

[14] F. Kiszkurno, J. Buchwald, O. Kolditz, T. Nagel.
Boom clay – a case study of the ATLAS in-situ full-scale heating experiment.
In *Geophysical Research Abstracts Vol. 25, EGU General Assembly*.
23–28 April, 2023, Vienna, Austria.

[15] A.A. Chaudhry, C. Zhang, O. Ernst, T. Nagel.
Effects of Inhomogeneity and Anisotropy on THM Simulations.
In *Geophysical Research Abstracts Vol. 25, EGU General Assembly*.
23–28 April, 2023, Vienna, Austria.

Output VIII

Output IX

Invited talks:

[1] T. Nagel, J. Buchwald, F. Kiszkurno, M. Pitz, D. Naumov, T. Helfer.
Navigating uncertainties in simulations of near- and far-field perturbations around underground excavations.
In *7th International Symposium on Tunnels and Shafts in Soils and Rocks. Session on Digital Analysis Tools*.
21 May, 2024, Mexico.

[2] T. Nagel, J. Buchwald, T. Helfer.
Hierarchical modelling in benchmarking, analysis and code development for coupled geo-processes.
In *94th Annual Meeting of the International Association of Applied Mathematics and Mechanics*.
19 Mar, 2024, Magdeburg, Germany.

[3] T. Nagel & MeQUR team.
Assessment of barrier integrity for nuclear waste repositories: THM modelling, software development and quantification of uncertainties.
In *EURECA-PRO seminar. 6. Priority Research Area Climate and environmental protection, modern energy. Research sub-area POB6.12: Nuclear energy*.
26 Apr, 2023, Poland (online).

Output X

[4] T. Nagel & MeQUR team.
Validated constitutive models in THMC process models: aspects of quality assurance in numerical safety analyses.
In *Institut Terre et Environnement de Strasbourg (ITES), Université de Strasbourg*.
16 Mar, 2023, Strasbourg, France.

[5] T. Nagel & MeQUR team.
Codes, process models and material knowledge: aspects of quality assurance in numerical safety analyses.
In *Model-based Development in Computational Engineering Seminar (RWTH Aachen)*
13 Jan, 2023, Aachen, Germany.

Theses:

[1] M. Poguntke.
Normalizing Flows – An Overview of Current Methods.
Masterarbeit. Fakultät für Mathematik. TU Chemnitz. März 2024.

[2] A.A. Chaudhry.
Sensitivity Analysis and Uncertainty Quantification of THM Simulations.
Dissertation. Fakultät für Geowissenschaften, Geotechnik und Bergbau. TU Bergakademie Freiberg. In preparation.

Output XI

[3] F. Kiszkurno.
Uncertainty Quantification and Model Selection in THM coupled simulations with cross-phenomenological fluxes.
Dissertation. Fakultät für Geowissenschaften, Geotechnik und Bergbau. TU Bergakademie Freiberg. In preparation.