HELMHOLTZ
Zentrum für Umweltforschung

Study on impact of thermo-osmosis on pressurisation

Hypothesis-testing and assisted-history-matching applied to evaluate uncertainty of model selection and parameter values

Feliks Kiszkurno

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Motivations and Research Questions

Motivation:

- Numerical models are used to prove integrity of nuclear waste repositories
- Decisions about assumptions, simplifications or expansion with additional processes can impact the results
- Thermo-osmosis (TO) is a relevant physical process for the nuclear waste storage

Research questions:

- Can TO be abused as a "tweaking parameter"?
- How does expansion with an arbitrary process impact the model uncertainty?

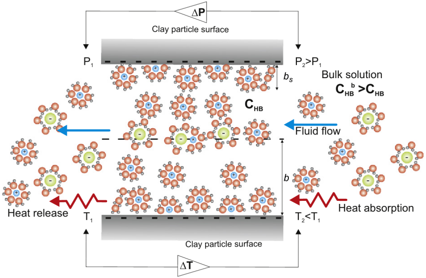


Figure: Schematic view of clay surface–pore fluid interactions. ([GMT12])

Physical processes - Mass balance equations

THM - Fully coupled Thermo-Hydro-Mechanical process

$$\underbrace{S_{\mathrm{THM}}\,\dot{p}}_{\text{Hydraulic storage}} \quad - \underbrace{\left[\phi_{\mathrm{F}}\beta_T^{\mathrm{L}} + 3\left(\alpha_{\mathrm{B}} - \phi_{\mathrm{F}}\right)\alpha_T^{\mathrm{S}}\right]\dot{T}}_{\text{Thermal storage}} + \underbrace{\alpha_{\mathrm{B}}\dot{u}_{i,i}}_{\text{Deformation}} + \underbrace{\left(w_{\mathrm{F}}\right)_{i,i}}_{\text{Fluid flow}} = \underbrace{Q_{\mathrm{H}}}_{\text{Sink/source}} \qquad (1)$$

$\mathrm{TH_{hyd}}$ - Thermo-Hydro process with correction term for the mechanical component

$$\left(S_{\mathrm{THM}} + \frac{\alpha_{\mathrm{B}}^2}{K_{\mathrm{S}}}\right)\dot{p} - \left(\beta_T^{\mathrm{eff}} - 3\alpha_{\mathrm{B}}\alpha_T^{\mathrm{S}}\right)\dot{T} + \left(w_{\mathrm{F}}\right)_{i,i} = 0 \qquad (2)$$

([Wan+21; Buc+21])

What is thermo-osmosis?

Definition:

"Thermo-osmosis may be defined as the process of diffusion of a fluid through a membrane under the influence of a temperature gradient" ([DR52; Gon+18])

How is TO added to the processes?

TO is included in the hydraulic flux component of the mass balance equations for THM and $\mathrm{TH_{hyd}}$:

$$\underbrace{(w_\mathrm{L})_i = -\frac{k_{ij}}{\mu_\mathrm{L}}\left(p_{,j} - \rho_\mathrm{L} g_j\right)}_{\text{original part}} - \underbrace{k_T T_{,i}}_{\text{thermo-osmosis}} \tag{3}$$

Thermo-osmosis - impact on pressure around the heater

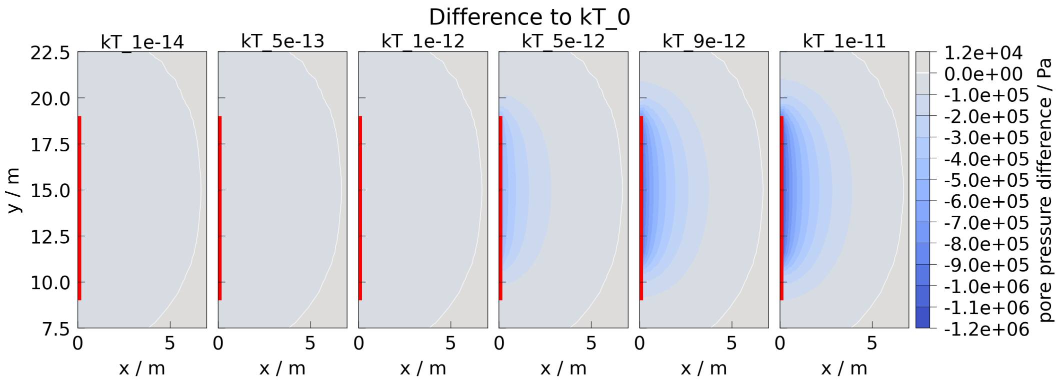


Figure: Red rectangle - heater. Difference to the reference data set without TO.

Impact of different TOC values

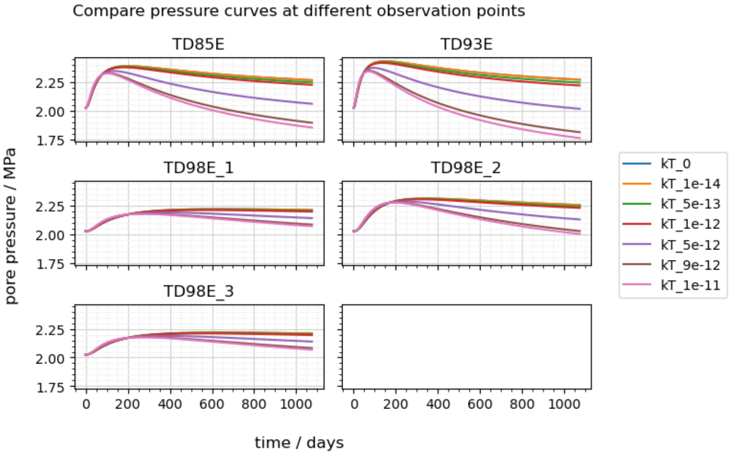
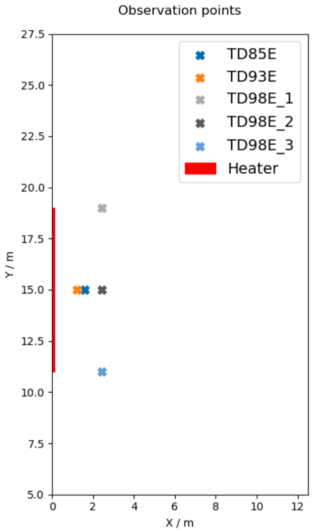


Figure: All tested TO coefficient values at different observation points.

- Impact of changing of TO coefficient value consistent between observation points
- Stronger at points closer to the heater

Experimental / Numerical Setup

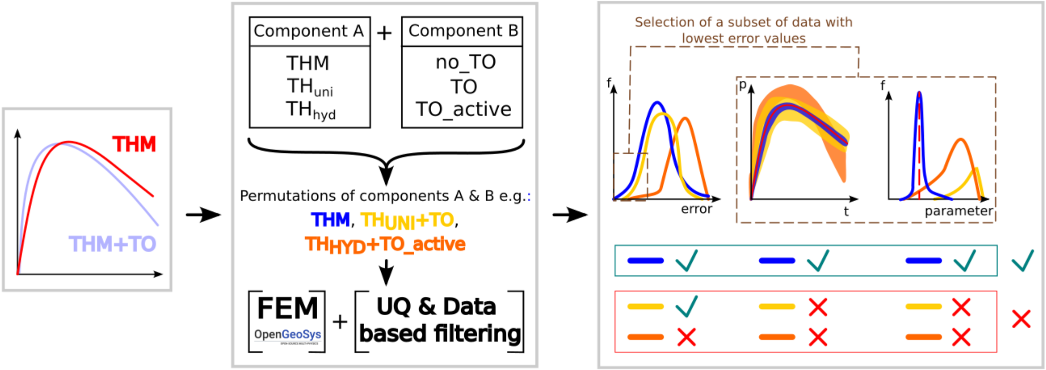


Variable name	Unit	Min. value	Max. value	Ref. value
Thermal expansivity (α_s)	K^{-1}	8×10^{-6}	2×10^{-5}	1.3×10^{-5}
Intrinsic permeability (k)	m^2	1×10^{-19}	9×10^{-19}	2.5×10^{-19}
Young's modulus (E)	Pa	2×10^{8}	8×10^{8}	3.5×10^{8}
Poisson's ratio (ν)	-	0.1	0.3	0.125
TO coefficient (wide)	$m^2\,s^{-1}\,K^{-1}$	1×10^{-14}	1×10^{-11}	3×10^{-12}
TO coefficient (active)	$m^2\,s^{-1}\,K^{-1}$	5×10^{-12}	1×10^{-12}	3×10^{-12}

Min. value – minimum value of parameter; Max. value – maximal value; Ref. value – reference value (used to obtain synthetic data)

- All observation points are located in the near field
- This study is based on but not identical with ATLAS III experiment ([Che+11; FLL09])
- Numerical simulations run with OpenGeoSys ([Bil+23])

Study idea / Workflow

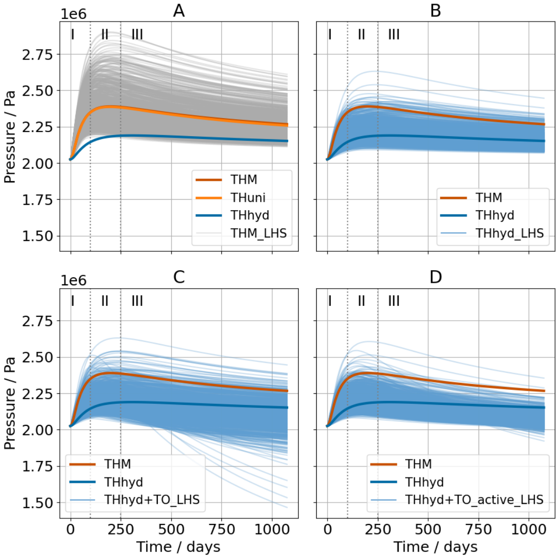


Select reference data set
E. g.: THM

Test different process variants

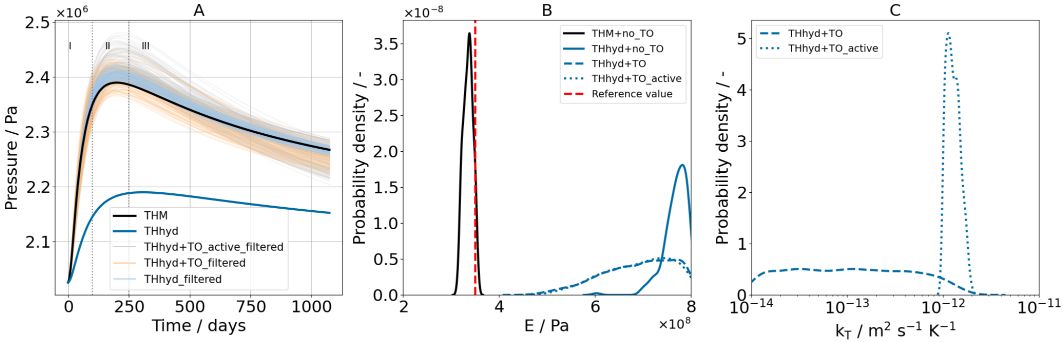
Ranking of process models

Less is more?



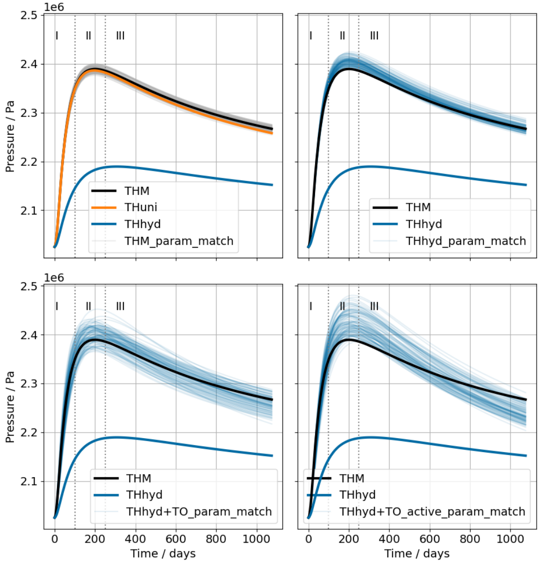
A
B
C
D
1e6
1e6
I
II
III
Pressure / Pa
2.75
2.50
2.25
2.00
1.75
1.50
0
250
500
750
1000
Time / days
THM
THuni
THhyd
THM_LHS
THhyd_LHS
THhyd+TO_LHS
THhyd+TO_active_LHS

Less is more?

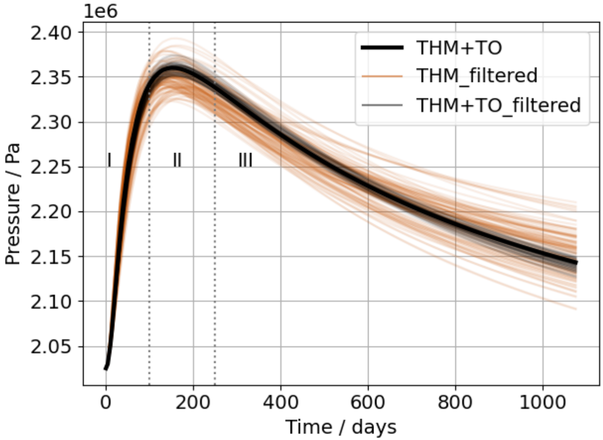


Out method doesn’t try to overfit the model by increasing its complexity!

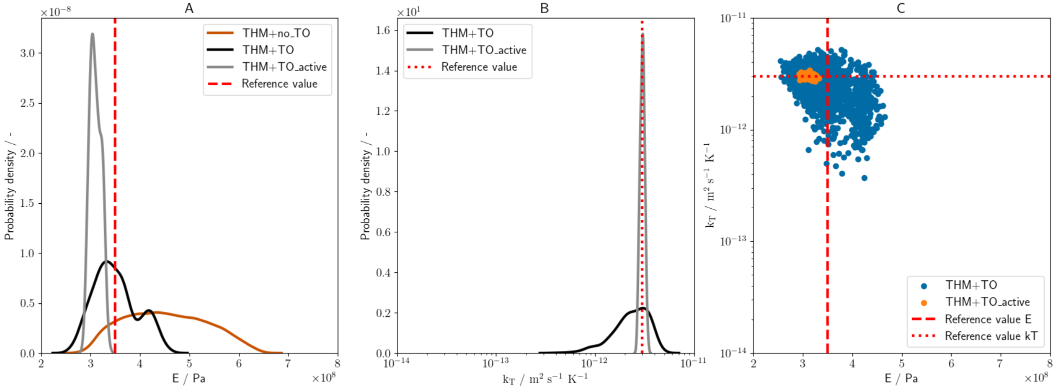
Less is more?


1e6
2.5
2.4
2.3
2.2
2.1
Pressure / Pa
I
II
III
THM
THuni
THhyd
THM_param_match
THM
THhyd
THhyd_param_match
1e6
THM
THhyd
THhyd+TO_param_match
THM
THhyd
THhyd+TO_active_param_match
0
200
400
600
800
1000
Time / days

What if TO is in the reference data?



What if TO is in the reference data?



Summary

Take-Home Messages

1. Adding a "tweaking parameter" without physical meaning doesn’t improve performance of the incorrect model
2. Presented workflow can choose correct level of model complexity
3. Increasing model complexity has to be backed by a physical justification

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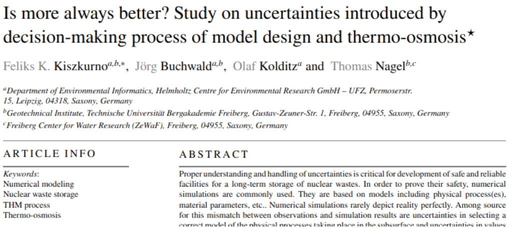
BGE BUNDESGESELLSCHAFT FÜR ENDLAGERUNG

URS Uncertainties and Robustness with regard to the Safety of a repository for high-level radioactive waste

OpenGeoSys OPEN-SOURCE MULTI-PHYSICS

Outlook



Is more always better? Study on uncertainties introduced by decision-making process of model design and thermo-osmosis*

Feliks K. Kiszkurno[a,b,*], Jörg Buchwald[a,b], Olaf Kolditz[a] and Thomas Nagel[b,c]

[a]Department of Environmental Informatics, Helmholtz Centre for Environmental Research GmbH – UFZ, Permoserstr. 15, Leipzig, 04318, Saxony, Germany
[b]Geotechnical Institute, Technische Universität Bergakademie Freiberg, Gustav-Zeuner-Str. 1, Freiberg, 04955, Saxony, Germany
[c]Freiberg Center for Water Research (ZeWaF), Freiberg, 04955, Saxony, Germany

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ABSTRACT

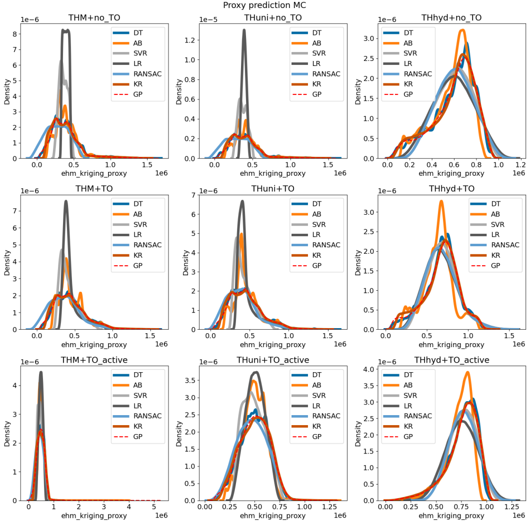
Proper understanding and handling of uncertainties is critical for development of safe and reliable facilities for a long-term storage of nuclear wastes. In order to prove their safety, numerical simulations are commonly used. They are based on models including physical process(es), material parameters, etc.. Numerical simulations rarely depict reality perfectly. Among source for this mismatch between observations and simulation results are uncertainties in selecting a correct model of the physical processes taking place in the subsurface and uncertainties in values

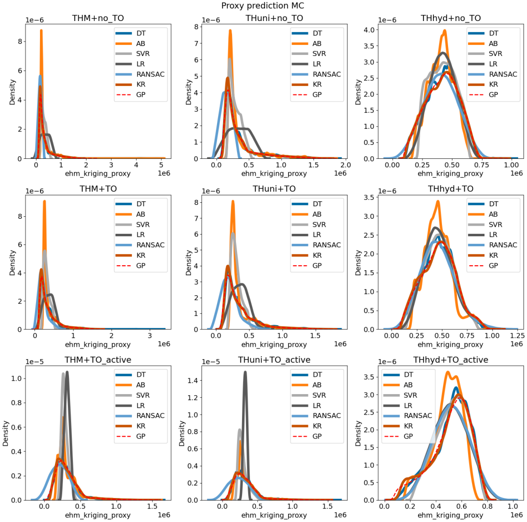
- Yay! First paper submitted to journal!

Next steps:

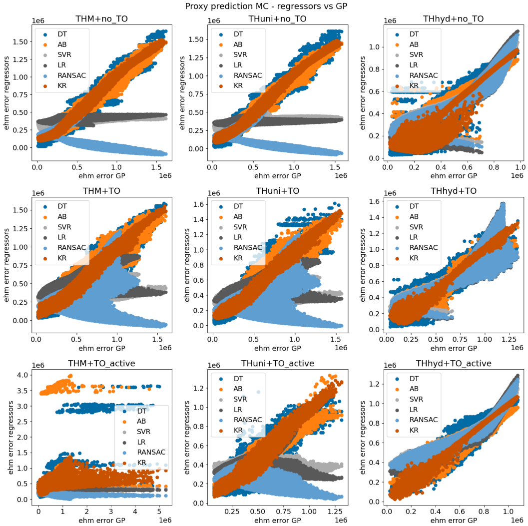
- Re-run the study on real data
  - ATLAS experiment
    - Anisotropy -> 3D?
  - TO experiment
    - 1D
    - [GT10]
- Test impact of the uncertainty on alternative algorithms used for proxy

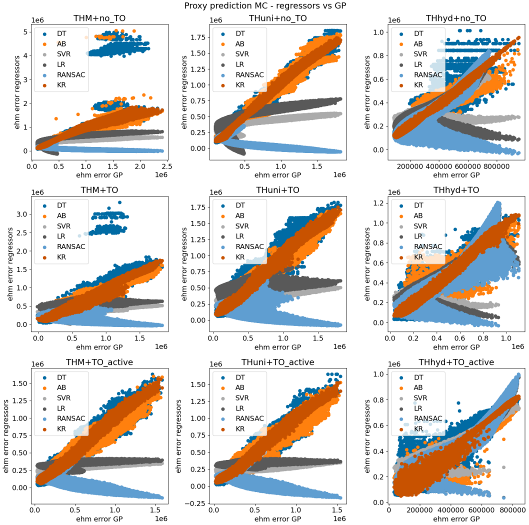
Outlook? - Proxy study



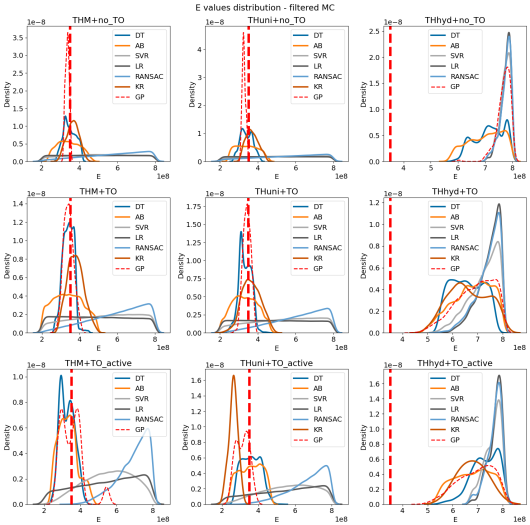


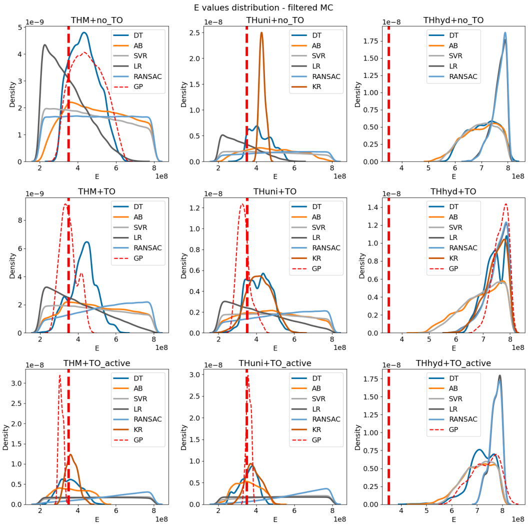
Outlook? - Proxy study



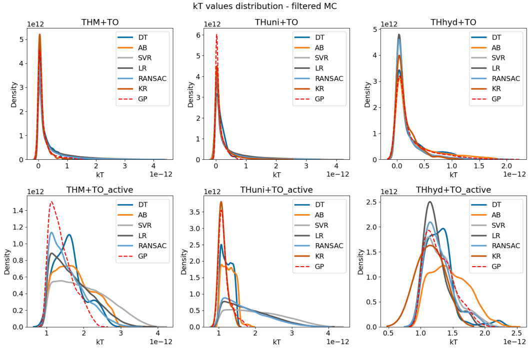


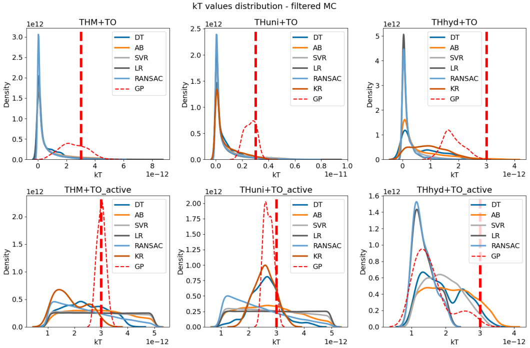
Outlook? - Proxy study





Outlook? - Proxy study





Thank you very much for your attention!

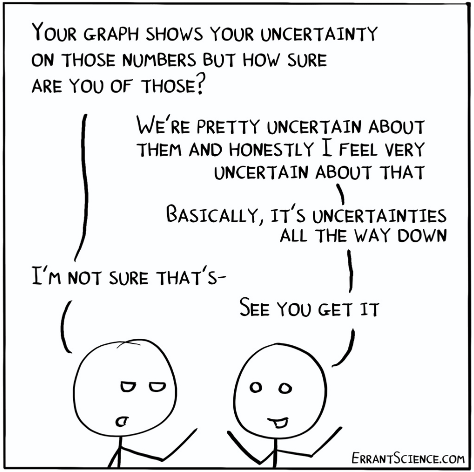


Figure: How NOT to handle uncertainties. (Author: ErrantScience.com)

Fun part! - URS Bear merch!

URS

Uncertainties and Robustness with regard to the Safety of a repository for high-level radioactive waste

We have a cool logo

-

let’s show it more!

Fun part! - URS Bear merch!

- Diameter: 50 mm
- Water resistant
- **Price: 30.75 €**

- Diameter: 53 mm
- **NOT** water resistant
- Short-term use
- Recyclable paper
- **Price: 37.25 €**

- Diameter: 20 mm
- Water resistant
- **Price: 74.75 €**

All prices are for 25 units.

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THM process

T - Thermal component - Energy balance equation

$$\underbrace{(\rho c_p)^{\text{eff}}\,\dot{T}}_{\text{Heat storage}} + \underbrace{\rho_{\text{F}}\, c_p^{\text{L}}\, T_{,i}\,(w_{\text{F}})_i}_{\text{Heat advection}} - \underbrace{\left(\lambda_T^{\text{eff}}\, T_{,i}\right)_{,i}}_{\text{Heat conduction}} = \underbrace{Q_T}_{\text{Heat source/sink}} \tag{4}$$

H - Hydraulic component - Mass balance equation

$$\underbrace{S_{\text{THM}}\,\dot{p}}_{\text{Hydraulic storage}} - \underbrace{\left[\phi_{\text{F}}\beta_T^{\text{L}} + 3\,(\alpha_{\text{B}} - \phi_{\text{F}})\,\alpha_T^{\text{S}}\right]\dot{T}}_{\text{Thermal storage}} + \underbrace{\alpha_{\text{B}}\,\dot{u}_{i,i}}_{\text{Deformation}} + \underbrace{(w_{\text{F}})_{i,i}}_{\text{Fluid flow}} = \underbrace{Q_{\text{H}}}_{\text{Sink/source}}, \tag{5}$$

M - Mechanical component - Momentum balance equation

$$\underbrace{\sigma_{ij,j}}_{\text{Total stress}} + \underbrace{\rho g_i}_{\text{Body force}} = 0 \tag{6}$$

([Wan+21; Buc+21])

Corrections: TH_{uni} vs TH_{hyd}

Storage term correction

$$\overbrace{\left(S_{THM} + \frac{\alpha_B^2}{K_S}\right)}^{C_{THhyd}} = \overbrace{\left(S_{THM} + \frac{\alpha_B^2}{E_S^S}\right)}^{C_{THuni}} \tag{7}$$

$$\overbrace{\frac{\phi}{K_F} + \frac{\alpha_B - \phi}{\frac{E^H}{3(1-2\nu^H)}} + \frac{\alpha_B^2}{\frac{E^H}{3(1-2\nu^H)}}}^{C_{THhyd}} = \overbrace{\frac{\phi}{K_F} + \frac{\alpha_B - \phi}{\frac{E^U}{3(1-2\nu^U)}} + \frac{\alpha_B^2}{\frac{E^U(1-\nu^U))}{(1+\nu^U)(1-2\nu^U)}}}^{C_{THuni}} \tag{8}$$

- Correction to both processes only depends on Young's Modulus (E^U and E^H) and Poisson's ratio (ν^U and ν^H)

Corrections: TH_{uni} vs TH_{hyd}

Temperature correction

$$\overbrace{\beta_T^{eff} - 3\alpha_B\alpha_S}^{C_{THhyd}} = \overbrace{\beta_T^{eff} - \alpha_B\alpha_S\frac{1+\nu}{1-\nu}}^{C_{THuni}} \tag{9}$$

$$\overbrace{\phi\beta_T^L + 3(\alpha_B - \phi)\alpha_S^H - 3\alpha_B\alpha_S^H}^{C_{THhyd}} = \overbrace{\phi\beta_T^L + 3(\alpha_B - \phi)\alpha_S^U - \alpha_B\alpha_S^U\frac{1+\nu^U}{1-\nu^U}}^{C_{THuni}} \tag{10}$$

- Correction to both processes only depends on Poisson's ratio (ν^U and ν^H) and thermal expansivity coefficient (α_S^U and ν_S^H)

Corrections: TH_{uni} vs TH_{hyd}

Storage term correction

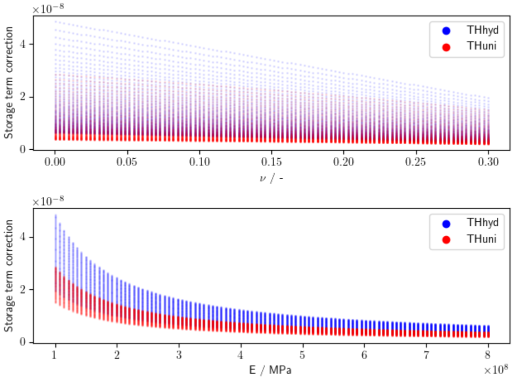

Figure: Overview of values of the storage correction depending on: Poisson's ratio (upper subfigure) and thermal Young's module (lower subfigure).

Corrections: TH_{uni} vs TH_{hyd}

Temperature correction

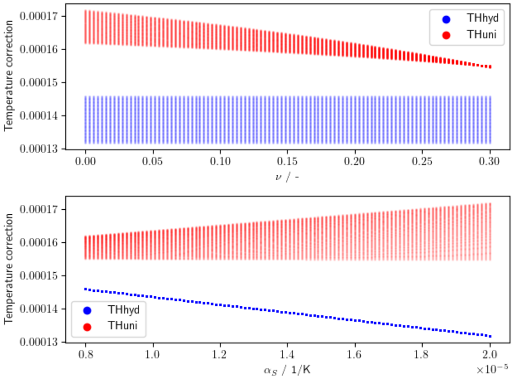

Figure: Overview of values of the expansivity correction depending on: Poisson's ratio (upper subfigure) and thermal expansivity coefficient (lower subfigure).

Impact of different TO coefficient values

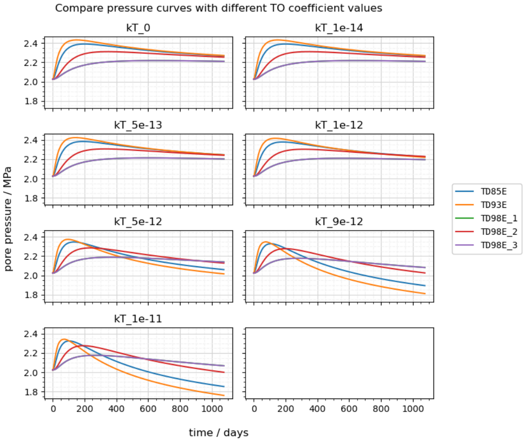

Figure: Pressure curves at all observation points for different values of TO coefficient.

- Regardless of value of TO coefficient the effect is strongest at points closest to the heat source