



Near Field – URL FE/ATLAS

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OUTLINE

DoE-based history matching

Parameter Uncertainties: FE-Experiment

Model Uncertainties: Thermo-Osmosis

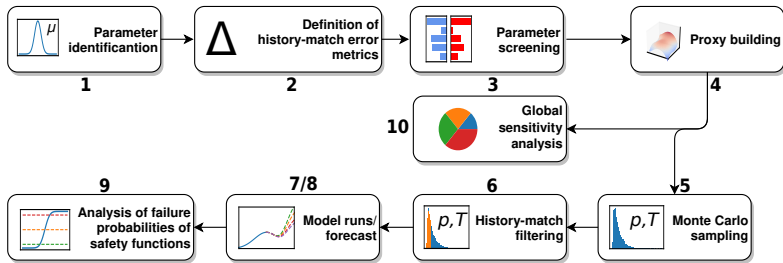
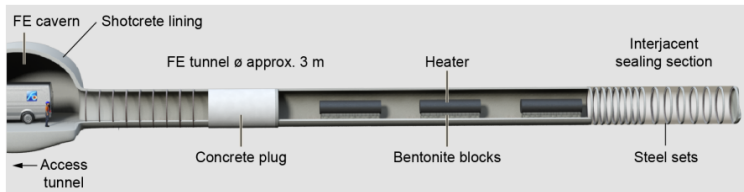


Fig. 1: Schematic sketch of the workflow. From Buchwald et al. 2020

- Workflow implemented in Python integrating a number of well-tested and own packages: pyDoE2, GPy, SALib, scipy, statsmodels, ChaosPy, ogsópy, vtk...
- workflow applied for treating **parameter uncertainties** (3D model of FE-experiment) and **model uncertainties** (thermos-osmosis in the ATLAS experiment)

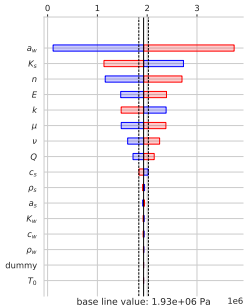


- Biggest heater experiment at Mt. Terri
- Modelled phases: excavation, shotcreting, emplacement, heating
- Parameter study for clay parameters on relative temperature and pressure changes in clay while heating
- Use of TH(m) model for forward runs (Buchwald et al. 2021).

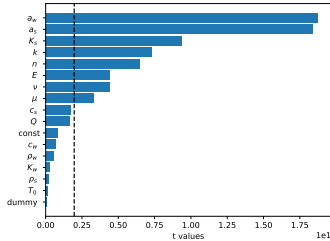
1. identifying parameter distributions, we restricted our analysis only to clay-related parameters
 - For clay 15-20 parameters; mostly min/best/max data available
 - uniform distributions were used
 - different resources → conflicting data
2. experiments (like the FE-Exp. at Mont Terri) allow for calibration/uncertainty reduction
 - use history-match error as objective function:

$$e^{\text{HM}} = \sqrt{\frac{1}{n} \sum_{i=1}^n (d_i^{\text{obs}} - d_i^{\text{sim}})^2}. \quad (1)$$

- used screening methods to identify heavy hitters/negligible parameters: one-variable-at-a-time, folded Plackett-Burman design to build Pareto charts



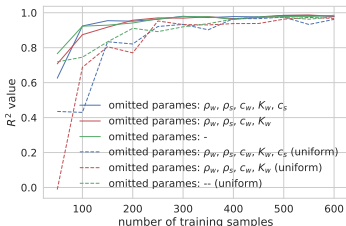
(a) OVAT tornado chart



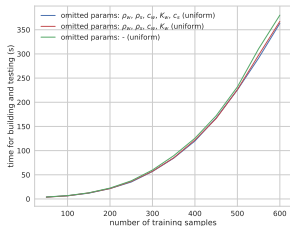
(b) PB Pareto chart

Fig. 2: Applied screening methods to temperature and pressure

4. Proxy building using Gaussian Process regression on a Latin-hypercube sampling plan



(a) R^2



(b) time for proxy building

Fig. 3: proxy quality measure and time for proxy building

5. Direct Monte-Carlo sampling on proxy

6. history-matching of Monte Carlo samples; thresholds based on proxy RMSE and subjective guesses for model error

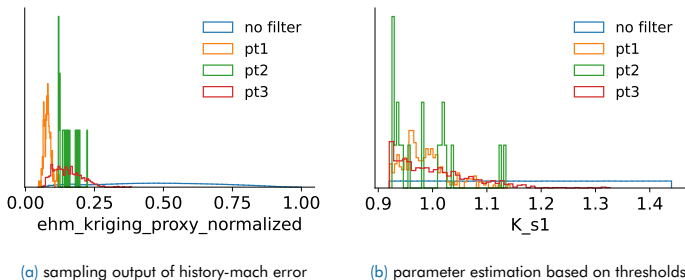
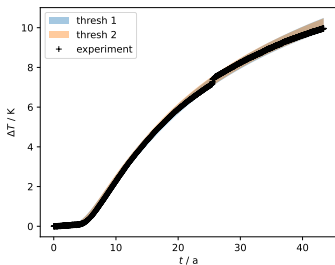
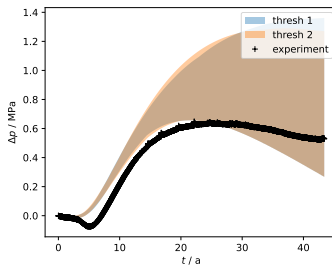


Fig. 4: History-Matching based on three different thresholds

7. forward model runs



(a) sampling output of history-mach error



(b) parameter estimation based on thresholds

Fig. 5: History-Matching based on three different thresholds

8. CDF based on last time step of response function

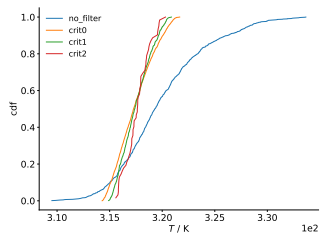


Fig. 6: CDF for temperature response

9. GSA based on Proxy

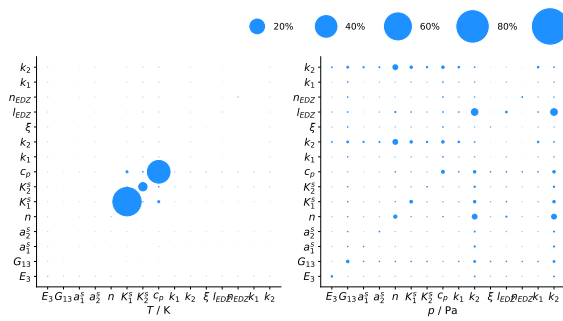


Fig. 7: first and second order Sobol indices

Main outcome

- temperatures can be matched very well
- Parameter uncertainties of other materials need to be considered as well
- features might be missing in the model or are not modeled well (geom. uncertainties, EDZ, etc.)

EQUATIONS

Mass balance

$$\frac{d_s}{dt} (\rho^w \varphi) + \nabla \cdot \mathbf{J}^w + \rho^w \varphi \nabla \cdot \frac{d_s \mathbf{u}}{dt} = q_w \quad (2)$$

where:

$$\mathbf{J}^w = -\rho^w \frac{\mathbf{k}_p}{\mu} (\nabla p - \rho^w \mathbf{g}) - \rho^w \mathbf{k}_{pT} \nabla T \quad (3)$$

Heat balance

$$\begin{aligned} \frac{d_s}{dt} ((C^s \rho^s (1 - \varphi) + C^w \rho^w \varphi) T) + \nabla \cdot \mathbf{i} + \\ + \nabla \cdot \mathbf{J}_E^w = q_E \end{aligned} \quad (4)$$

where:

$$\mathbf{i} = -(\mathbf{K}^s (1 - \varphi) + \mathbf{K}^w \varphi) \nabla T - T \mathbf{k}_{pT} \nabla p \quad (5)$$

and

$$\mathbf{J}_E^w = C^w \rho^w \mathbf{v}^w \quad (6)$$

In all equations above \mathbf{k}_{pT} is thermo-osmosis tensor. Zhigang 2020

OVERVIEW

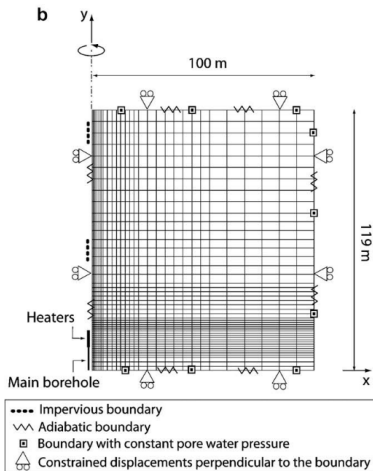
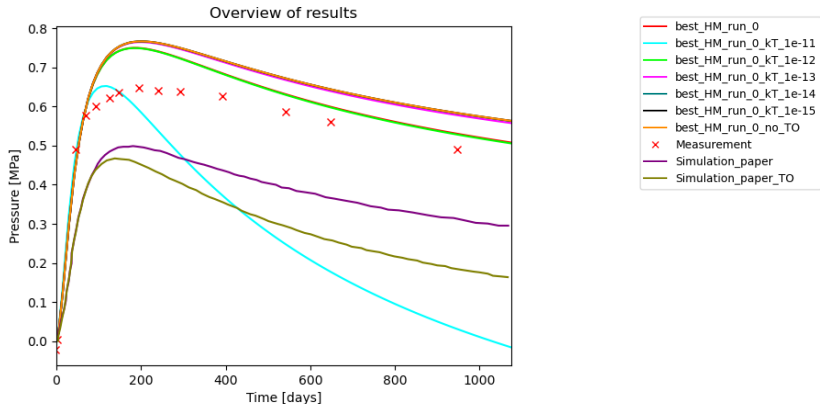


Fig. 8: Layout of ATLAS Experiment. Figure from: François, Laloui, and Laurent 2009

THE EFFECT OF K_T



OVERVIEW

Tested parameter ranges

Parameter name	Unit	Reference	Min	Max
Thermal expansivity (α_s)	K^{-1}	$1.3e - 5$	$5e - 5$	$5e - 3$
Intrinsic permeability (k)	m^2	$2.5e - 19$	$8e - 20$	$4e - 19$
Thermoosmosis coefficient (k_T)	$Pa * m * K^{-1}$	-	$1e - 13$	$9e - 13$
Young's modulus (E)	MPa	$3.5e8$	$3e8$	$6e8$
Poissons ratio (ν)	-	0.125	0.1	0.15

Reference values after: Tamizdoust and Omid Ghasemi-Fare 2021.

Initial conditions:

Parameters	Values	Units
$\sigma_x = \sigma_y$	4.5	MPa
p_0	2.025	MPa
T_0	16.5	$^{\circ}C$

Initial conditions after: Tamizdoust and Omid Ghasemi-Fare 2021.

Error metrics

$$e_{HM} = \sum_1^n \frac{(d_{obs} - d_{sim})^2}{n} \quad (7)$$

P AND T CURVES

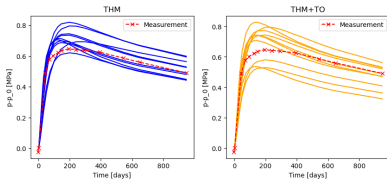


Fig. 9: Porepressure at observation point.

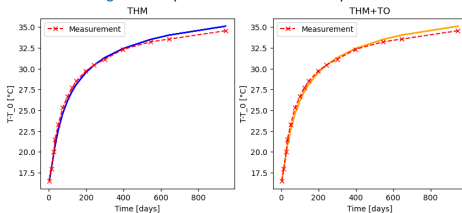


Fig. 10: Temperature at observation point.

PARAMETER ESTIMATION

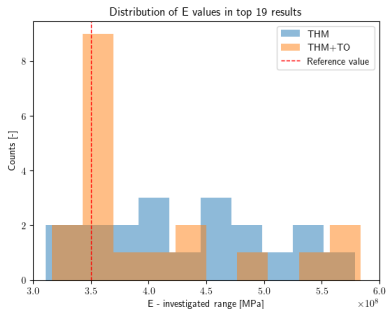


Fig. 11: Young's modulus.

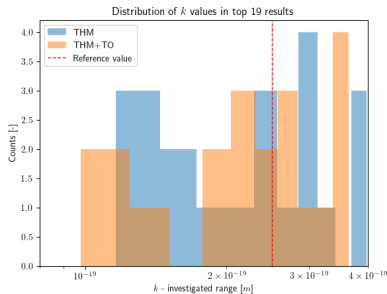


Fig. 12: Intrinsic permeability.

EHM - DISTRIBUTIONS

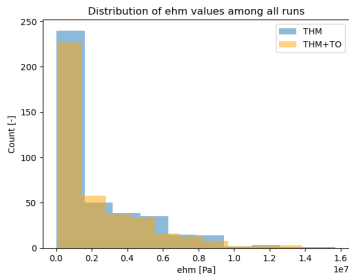


Fig. 13: Entire ehm range.

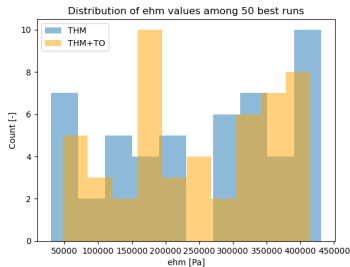


Fig. 14: Zoom-in to best runs.

Main outcomes:

- temperatures are matched very well
- No clear improvement visible by consideration of TO-effect.
- further refinements might be need
- features might be missing that could improve both matches (anisotropy)

- FE modelling Taskforce
- iCross Project
- OpenWorkFlow project



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REFERENCES

- [1] J Buchwald et al. "DoE-based history matching for probabilistic uncertainty quantification of thermo-hydro-mechanical processes around heat sources in clay rocks". In: *International Journal of Rock Mechanics and Mining Sciences* 134 (2020), p. 104481.
- [2] J Buchwald et al. "Improved predictions of thermal fluid pressurization in hydro-thermal models based on consistent incorporation of thermo-mechanical effects in anisotropic porous media". In: *International Journal of Heat and Mass Transfer* 172 (2021), p. 121127.
- [3] Bertrand François, Lyesse Laloui, and Clément Laurent. "Thermo-Hydro-Mechanical Simulation of ATLAS in Situ Large Scale Test in Boom Clay". In: *Computers and Geotechnics* 36.4 (May 1, 2009), pp. 626–640. ISSN: 0266-352X. DOI: 10.1016/j.compgeo.2008.09.004. URL: <https://www.sciencedirect.com/science/article/pii/S0266352X08001109> (visited on 07/14/2022).

REFERENCES II

- [4] Mohammadreza Mir Tamizdoust and Omid Ghasemi-Fare. “Assessment of Thermo-Osmosis Effect on Thermal Pressurization in Saturated Porous Media”. In: *IFCEE 2021*. International Foundations Congress and Equipment Expo 2021. Dallas, Texas, 2021, pp. 99–108. DOI: 10.1061/9780784483428.011. eprint: <https://ascelibrary.org/doi/pdf/10.1061/9780784483428.011>. URL: liquid.
- [5] Ye Zhiqiang. *Derivation and Verification of Governing Equations in a THM Model Considering Thermo-Osmosis and Thermo-Filtration Effects*. Oct. 19, 2020. URL: https://gitlab.opengeosys.org/ogs/ogs/-/raw/master/Tests/Data/ThermoHydroMechanics/Linear/CylindricalCavity/Docu_THM_thermo_osmosis_and_thermo_filtration.pdf?inline=false (visited on 03/30/2022).