energi SIMULATION

Building Confidence on Simulation of Salt Caverns for Energy Storage

Multiscale Experimental-Numerical, from Lab to Field

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15 October 2024, TNO Utrecht

TU Delft

A cavern ‘structure’ collapse → Sinkhole of 30m wide, 4.5m deep

Caves&Waves Project (Naomi van den Ameele et al.): risks of scaling up caverns for UHS

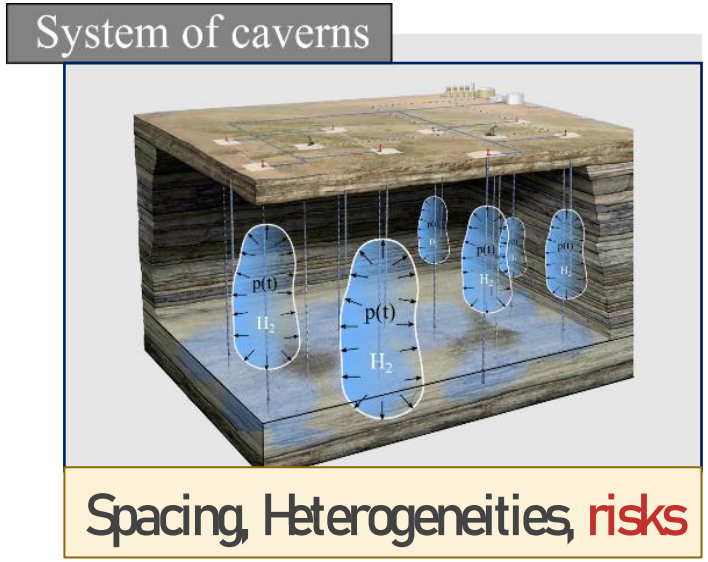
gasunie
crossing borders in energy

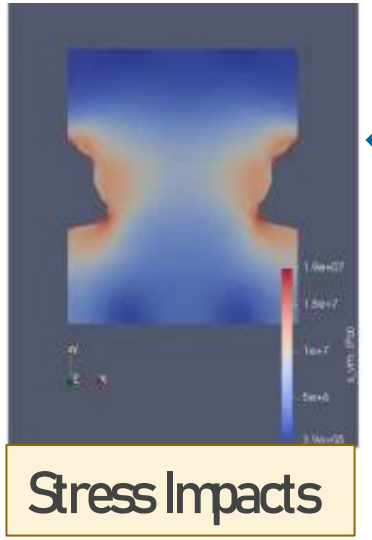
Scaling up salt caverns for energy storage: how safe & confident can/should we be?

GasUnie website

Salt Caverns for (H2) Cyclic Energy Storage: system caverns

- Dome-scale heterogeneities / caverns stability
- Nearby faults & weakness zones & subsidence
- System Cyclic Operations
- Caverns connectivity
- Scaled up ‘risks’
- Monitoring, Uncertainty reduction
- Design: Spacing, Volumes, …
- …

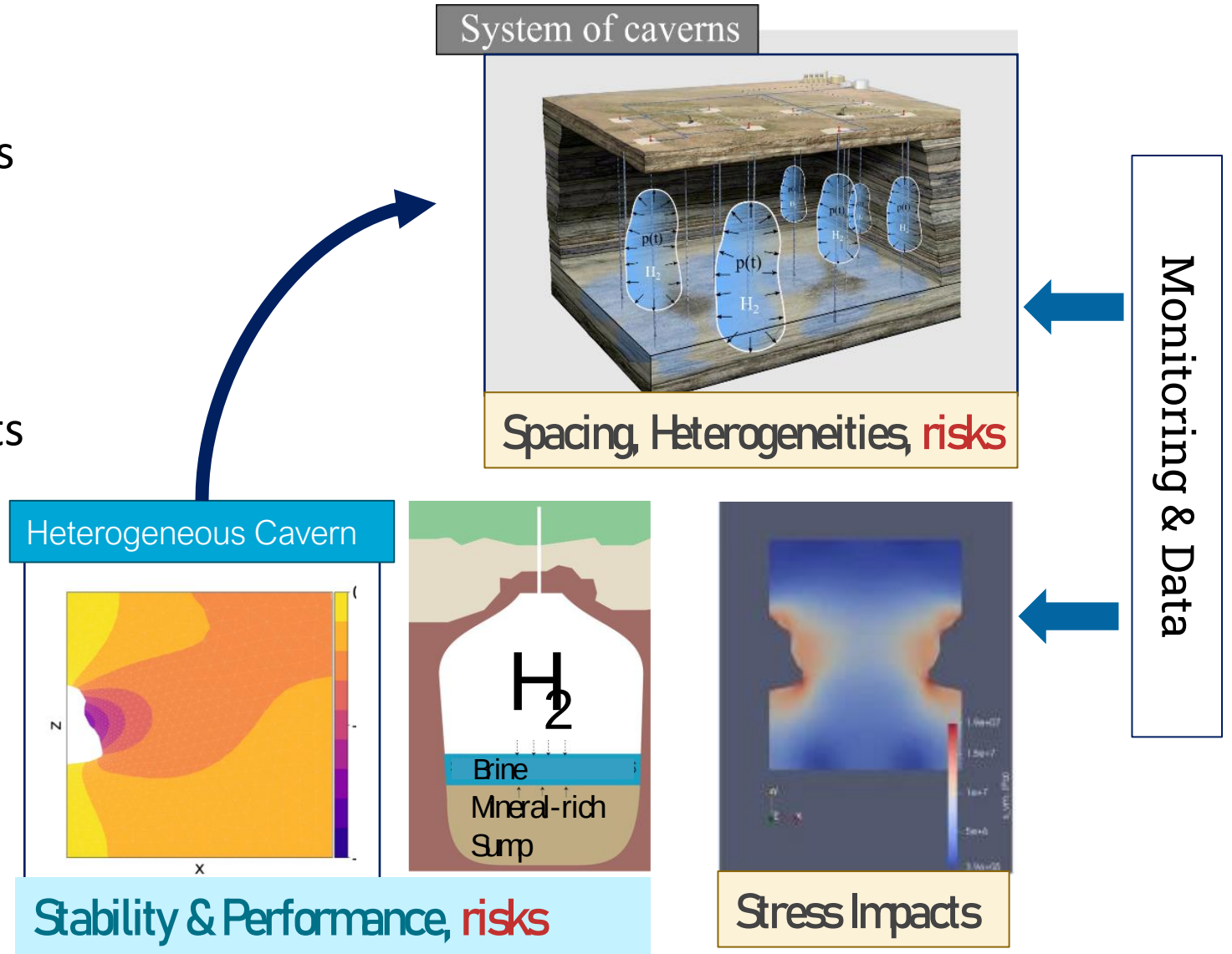




Monitoring & Data

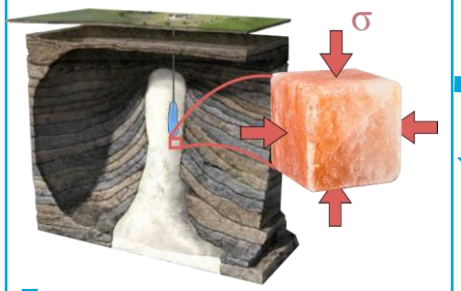
Salt Caverns for (H2) Cyclic Energy Storage: 1 cavern

- Heterogeneities, complex geometries
- Structural stability, subsidence, …
- Near well-bore stability
- Bio-geochemistry & exposure impacts (new or old for H2)
- Abandonment & Monitoring, …

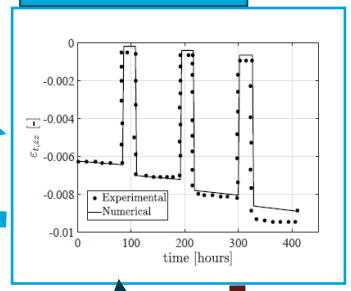


Salt Caverns for (H2) Cyclic Energy Storage: rock mechanics

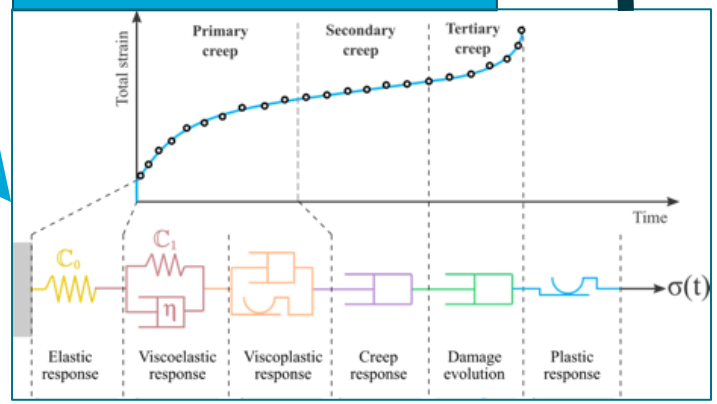
LAB



Validation

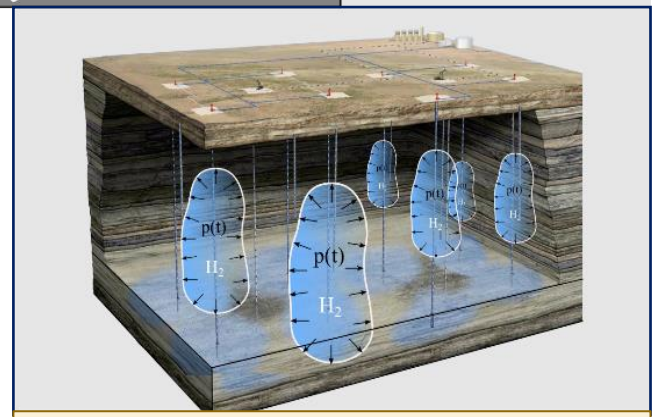


Constitutive Laws



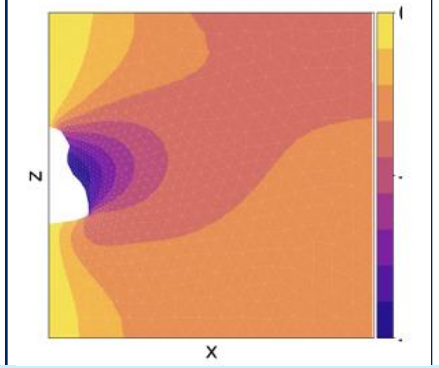
Mechanics Model & Parameter Calibration

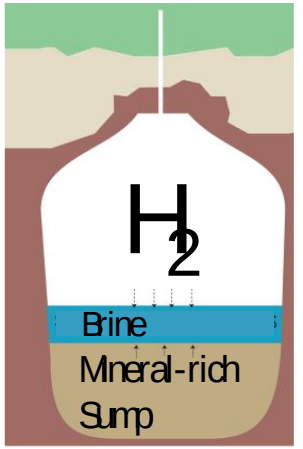
System of caverns



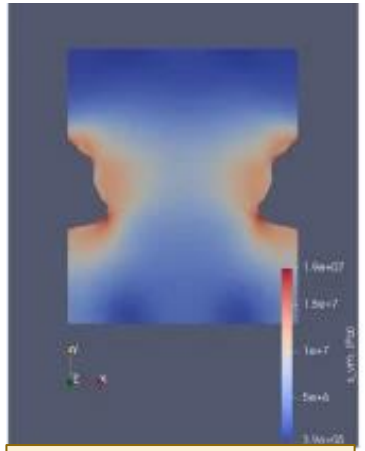
Spacing, Heterogeneities, risks

Heterogeneous Cavern





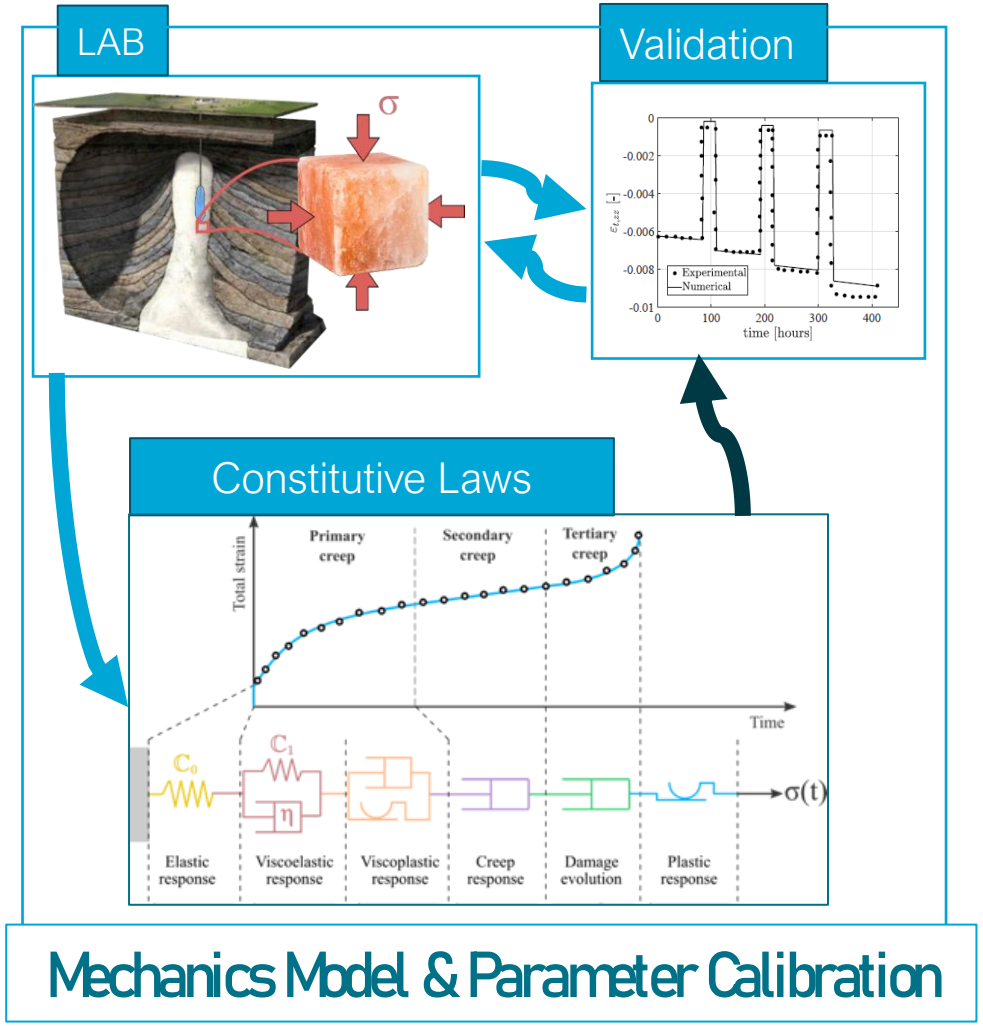
Stability & Performance, risks



Stress Impacts

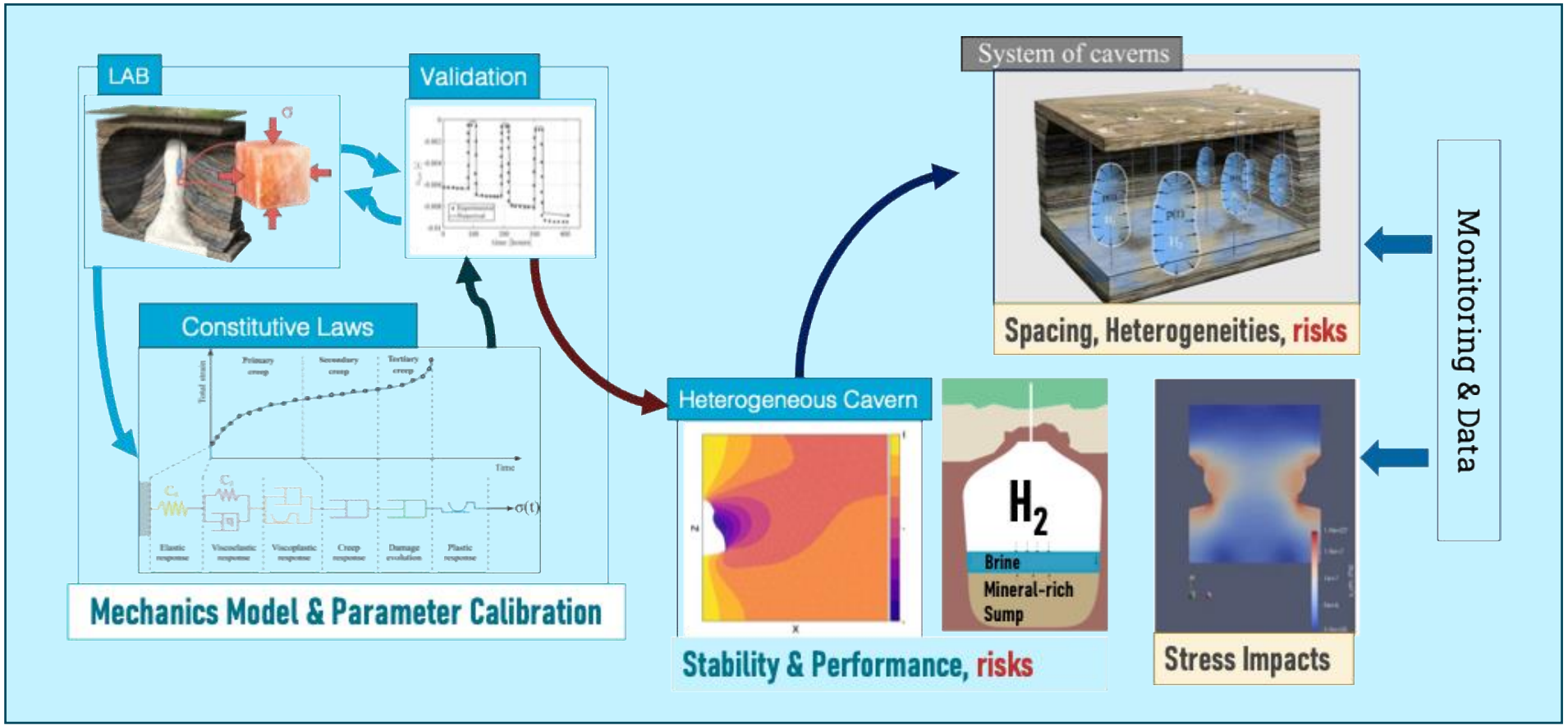
Monitoring & Data

Salt Caverns for (H2) Cyclic Energy Storage: rock mechanics



- Model selection & Parameter Calibration
- Challenges:
  - High quality 'relevant' experiments
  - Heterogeneous rocks?
  - Many models, or yet a new one?
  - Full-physics contains many mechanisms!
  - Too many parameters to calibrate, how to be predictable?

Salt Caverns for (H2) Cyclic Energy Storage: rock mechanics

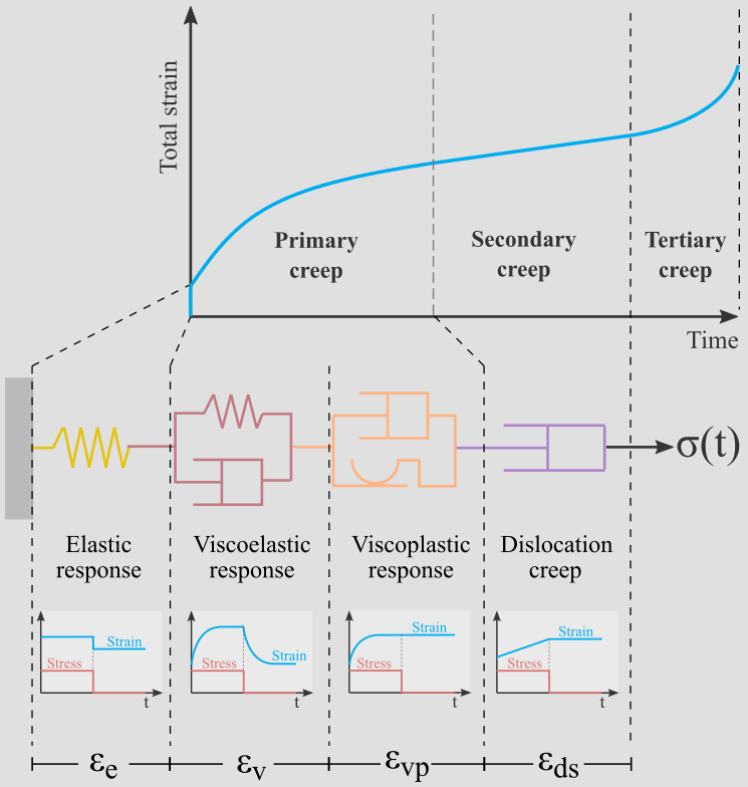


SAFEINCAVE

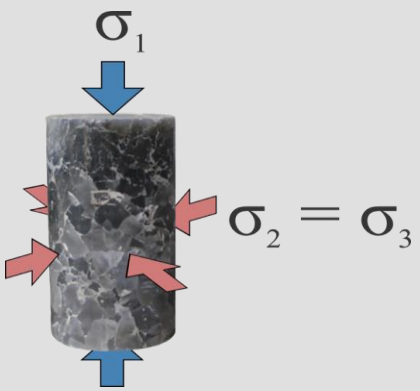
Open-Source Simulator for forward & inverse modeling:
Calibrate, Simulate, Optimize

Model Selection & Parameter Calibration

Constitutive model



Rock Under Load

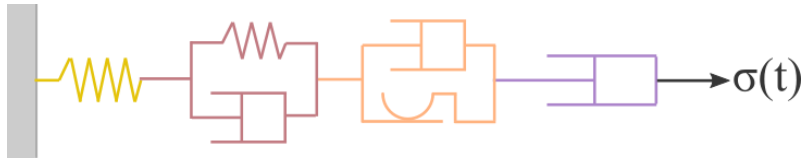


$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{bmatrix}$$

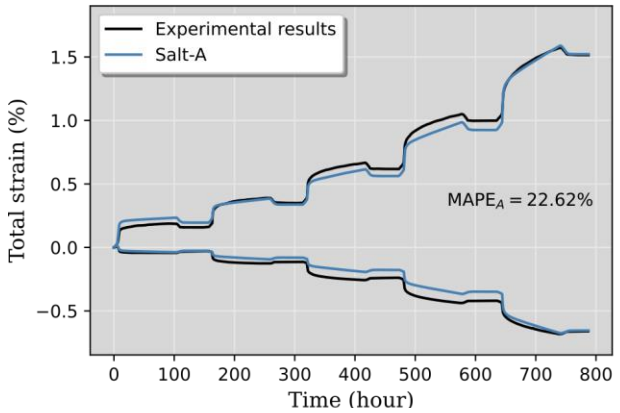
$$\boldsymbol{\varepsilon} = F(\boldsymbol{\sigma}, \mathbf{k})$$

Hermínio Tasinafo Honório et al. https://doi.org/10.1016/j.ijrmms.2024.105922 (2024)

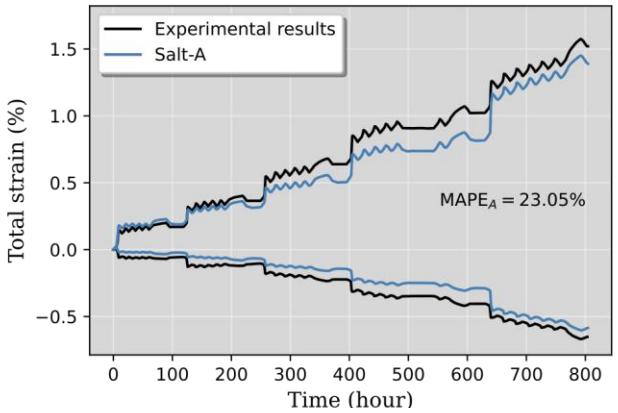
Model Selection & Parameter Calibration



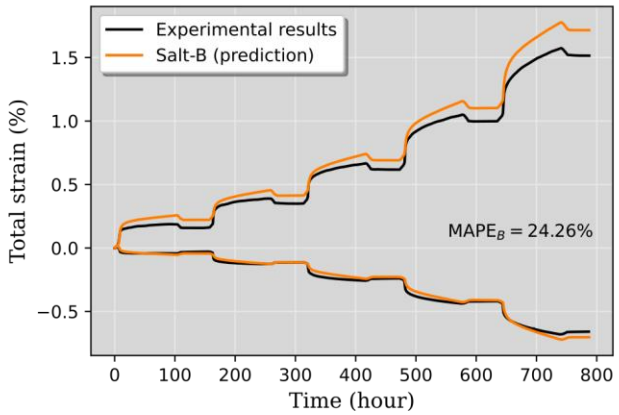
Test1



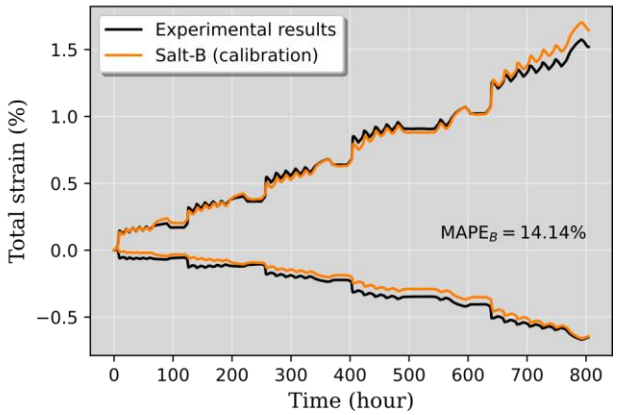
Test2



Test1

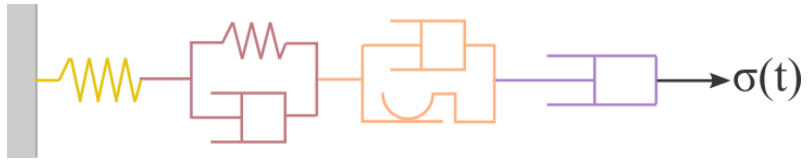


Test2

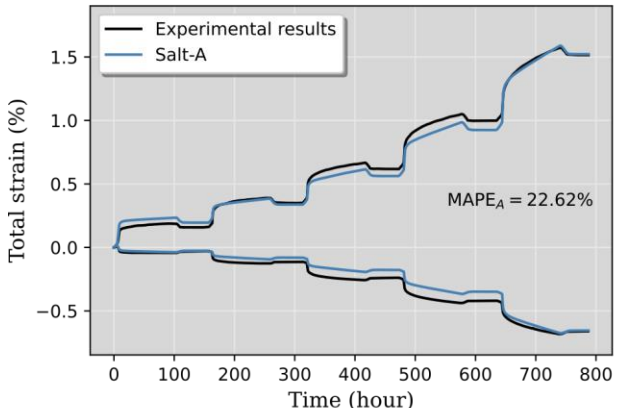


- 2 experiments on similar samples!
- Calibrating **k** with Test1 is not predictive for Test 2! & vice versa
- How do we reliably calibrate **k**?

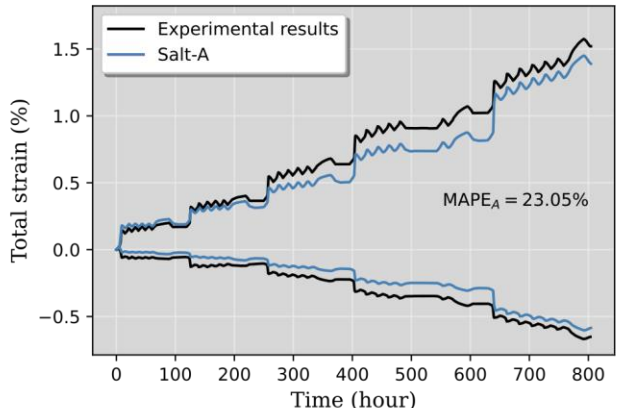
Model Selection & Parameter Calibration



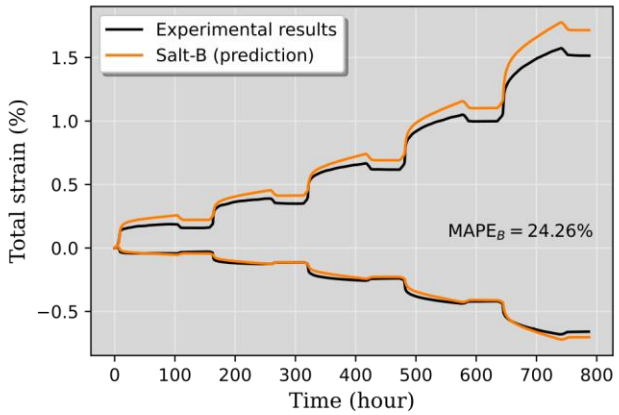
Test1



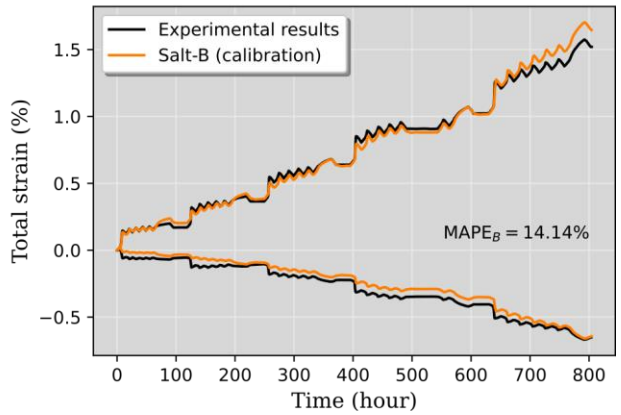
Test2



Test1



Test2



- 2 experiments on similar samples!
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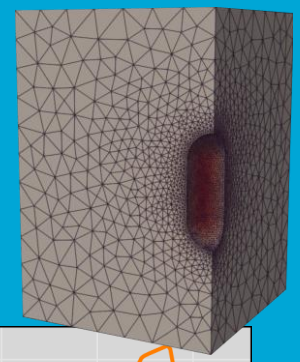
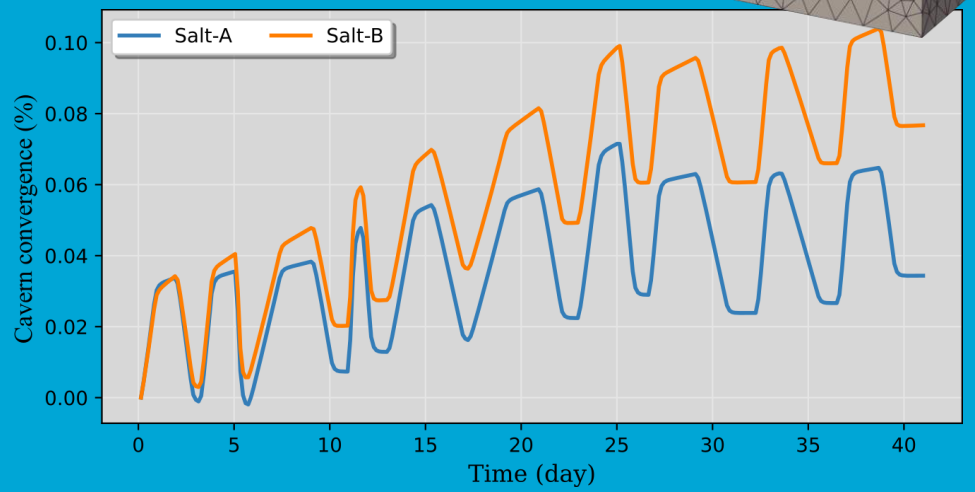
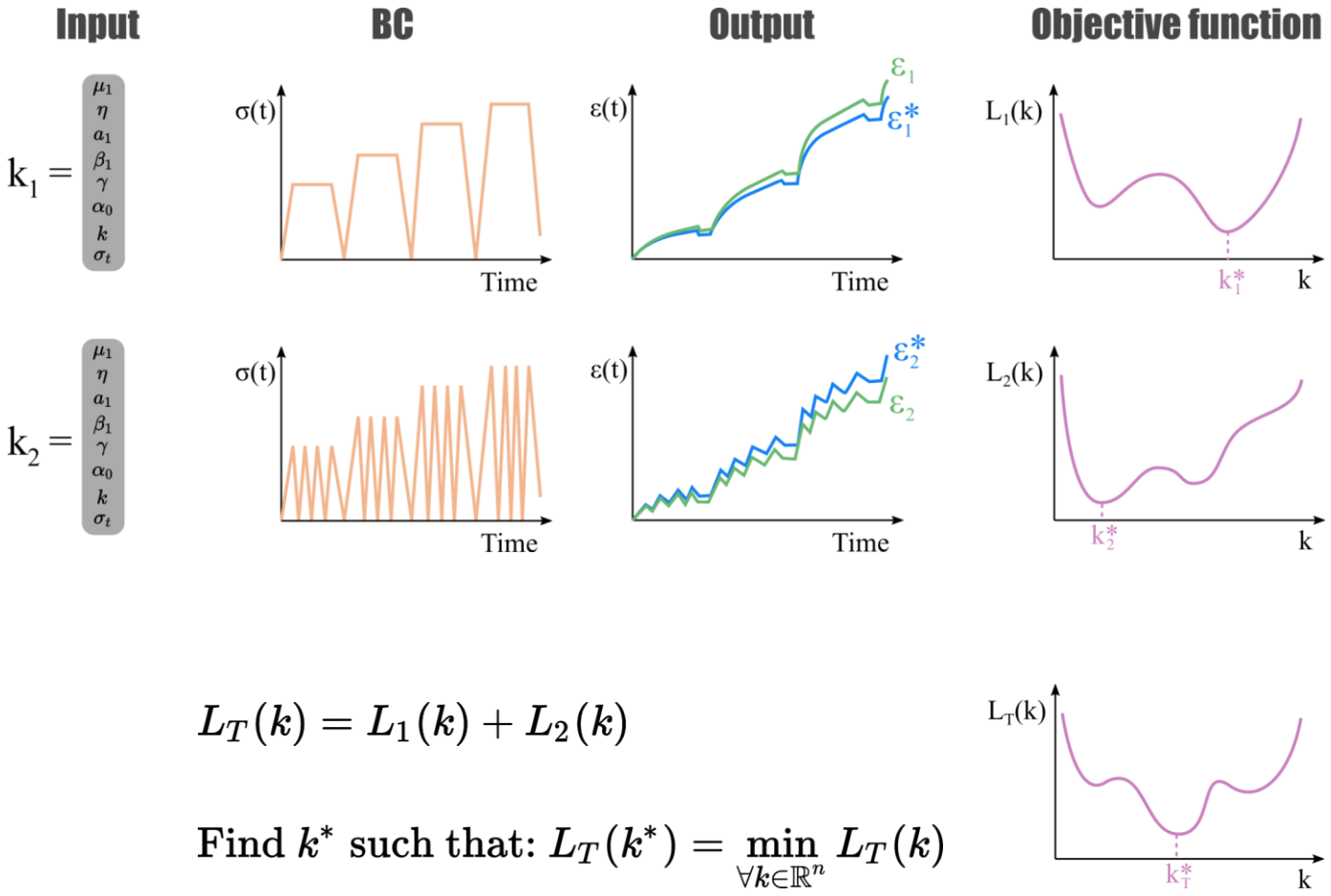
- How do we reliably calibrate **k**?





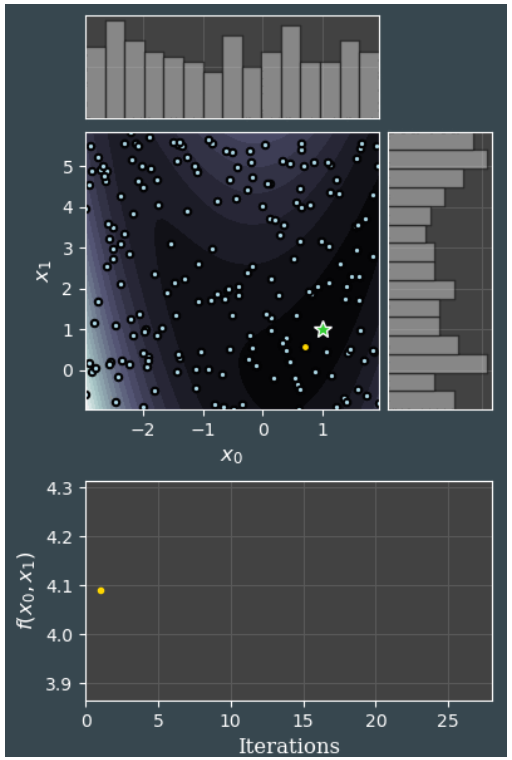
Significantly different results at cavern scale!

Model Selection & Parameter Calibration



$$L_T(k) = L_1(k) + L_2(k)$$

$$\text{Find } k^* \text{ such that: } L_T(k^*) = \min_{\forall k \in \mathbb{R}^n} L_T(k)$$

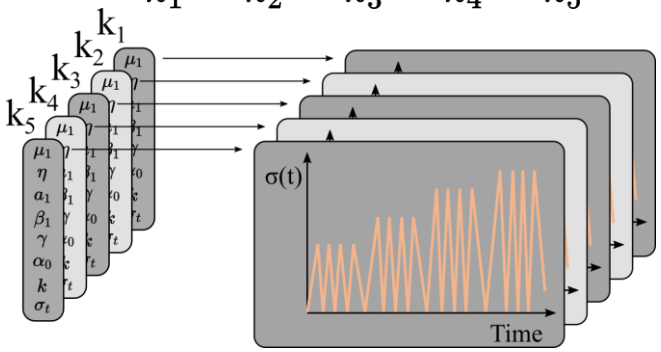


Particle Swarm Optimization

Hermínio Tasinafo Honório et al. https://doi.org/10.1016/j.ijrmms.2024.105922 (2024)

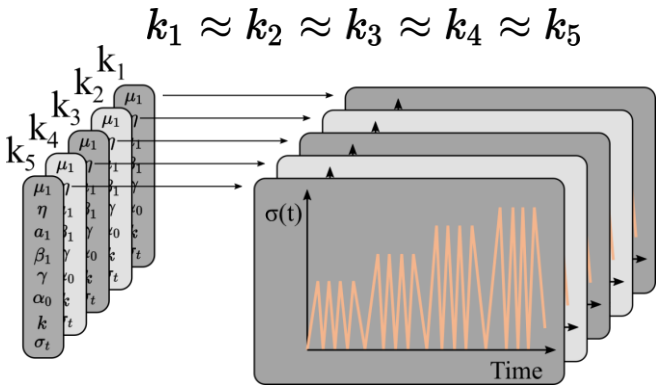
Test: Model known, parameters uncertain

$$k_1 \approx k_2 \approx k_3 \approx k_4 \approx k_5$$

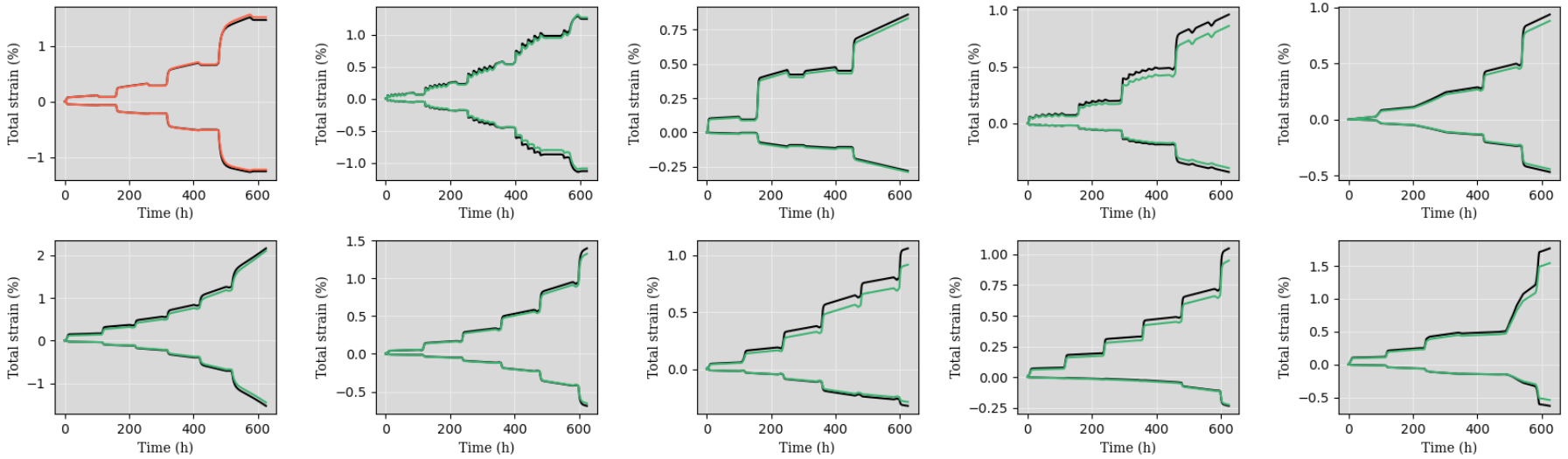


Model uncertainty: NO
Property uncertainties: YES

Test: Model known, parameters uncertain

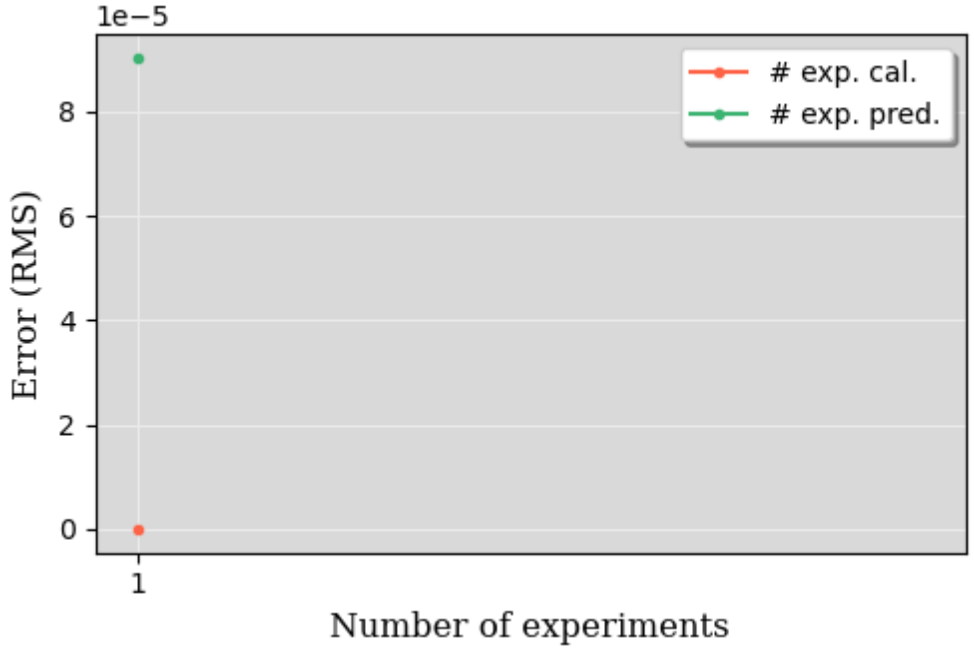


Model uncertainty: NO
Property uncertainties: YES

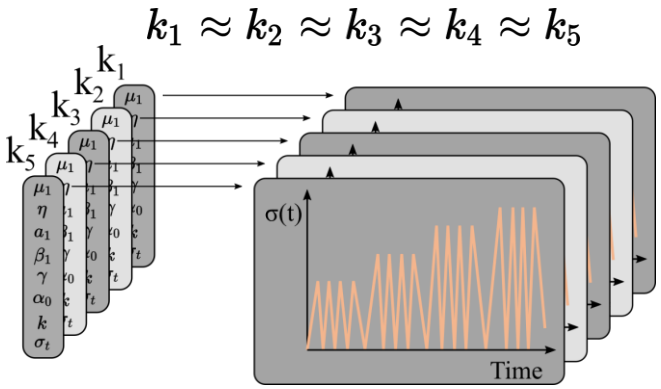


Calibration

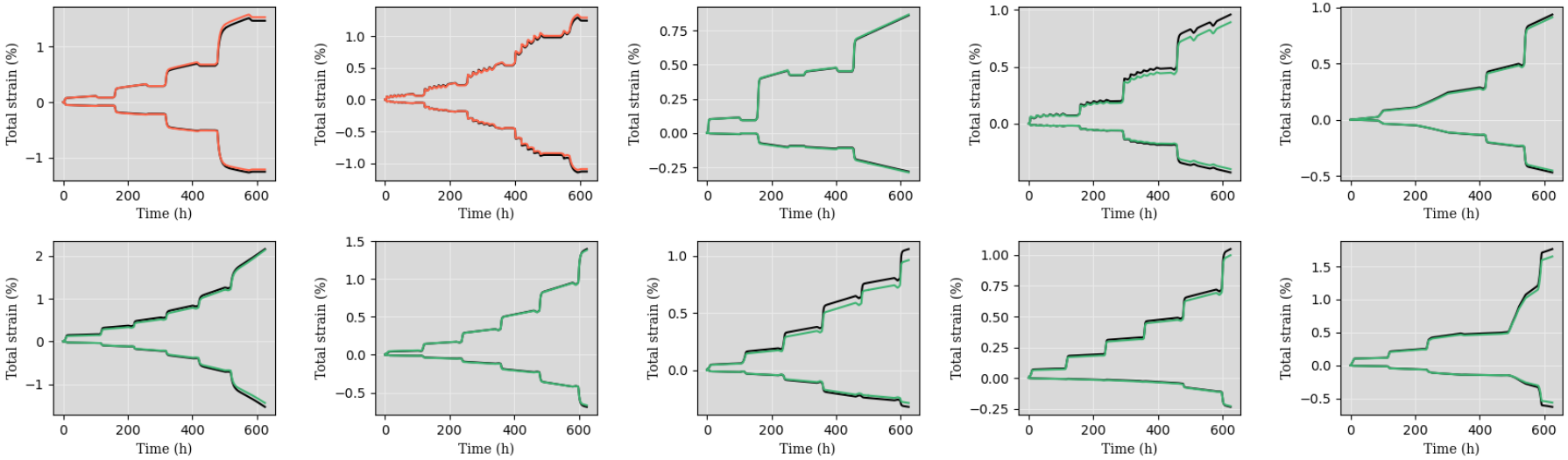
Prediction



Test: Model known, parameters uncertain

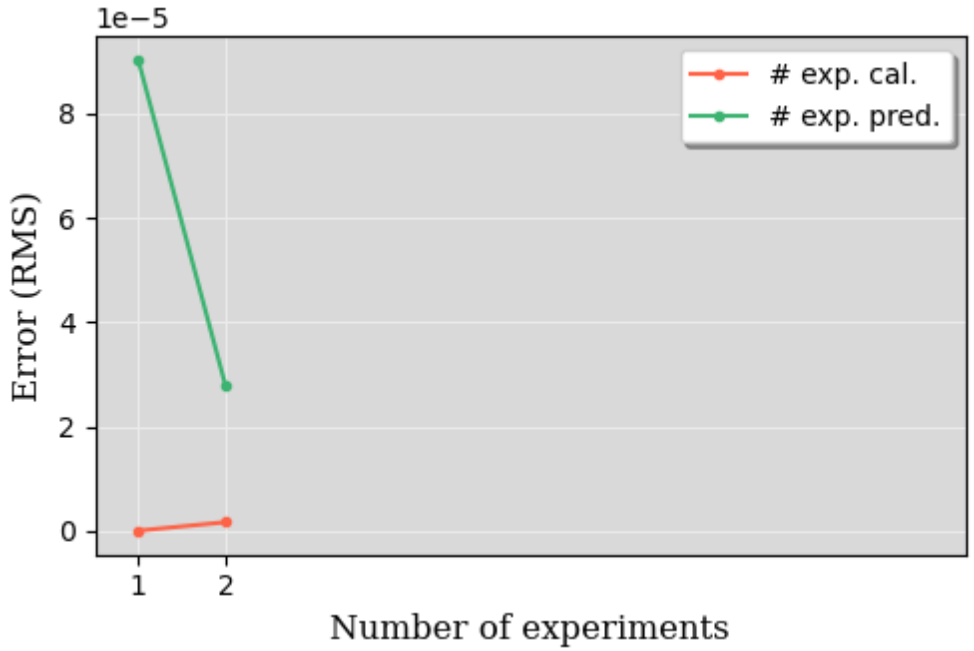


Model uncertainty: NO
Property uncertainties: YES

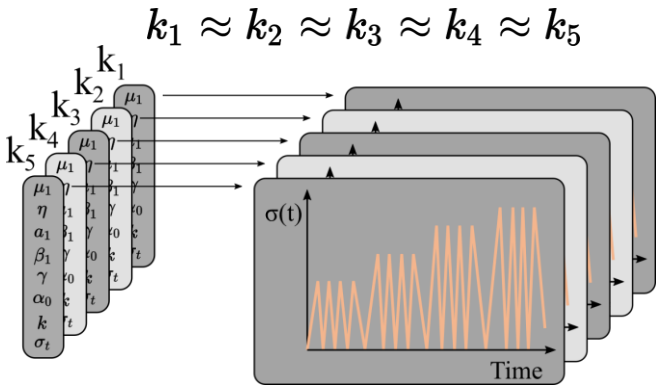


Calibration

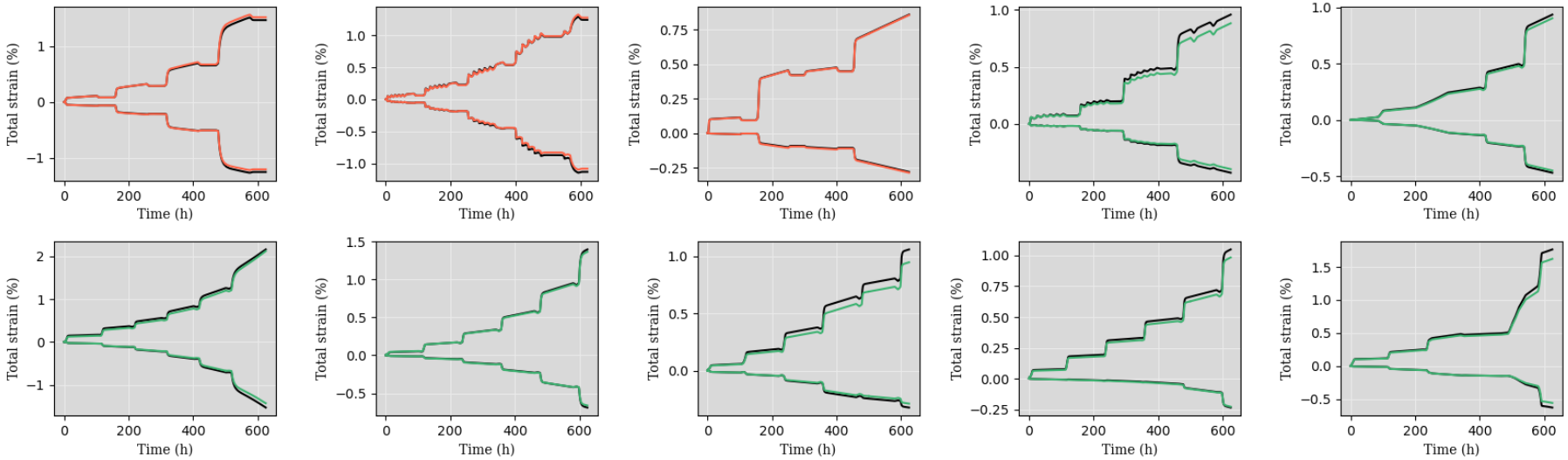
Prediction



Test: Model known, parameters uncertain



Model uncertainty: NO
Property uncertainties: YES



Calibration

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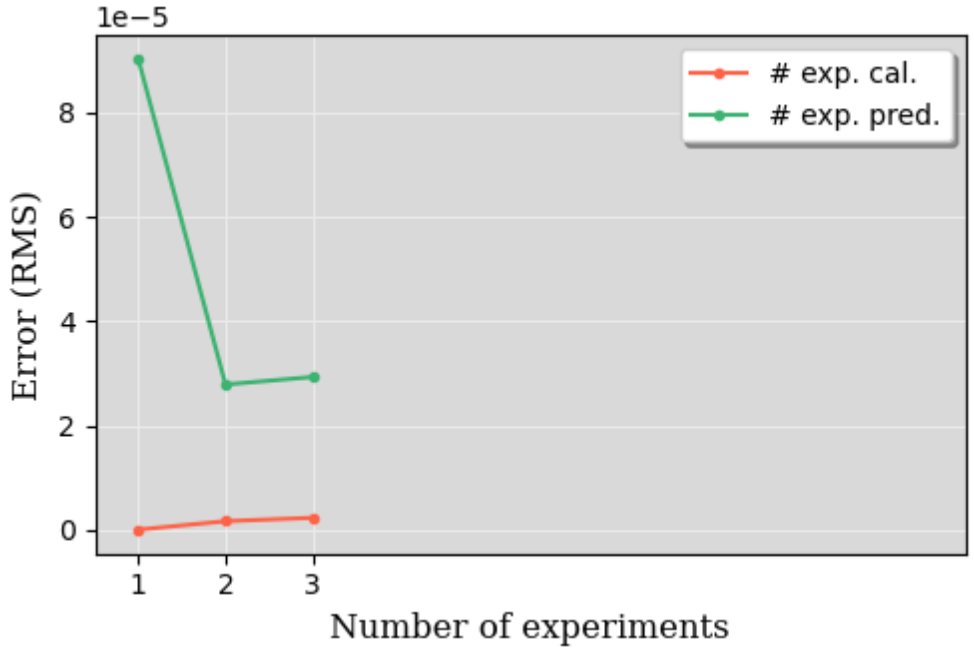
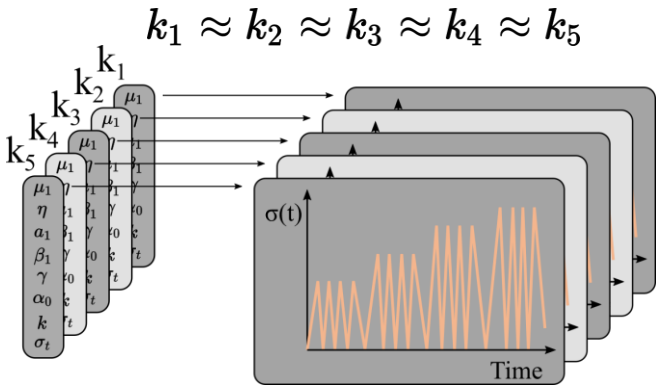


Test: Model known, parameters uncertain



Model uncertainty: NO
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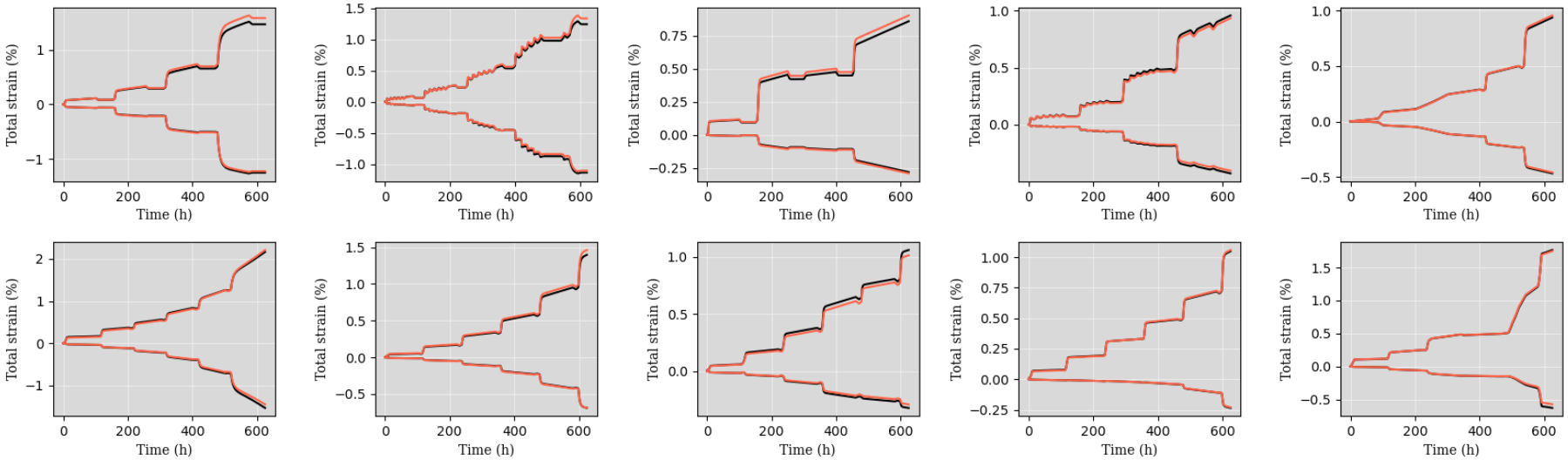
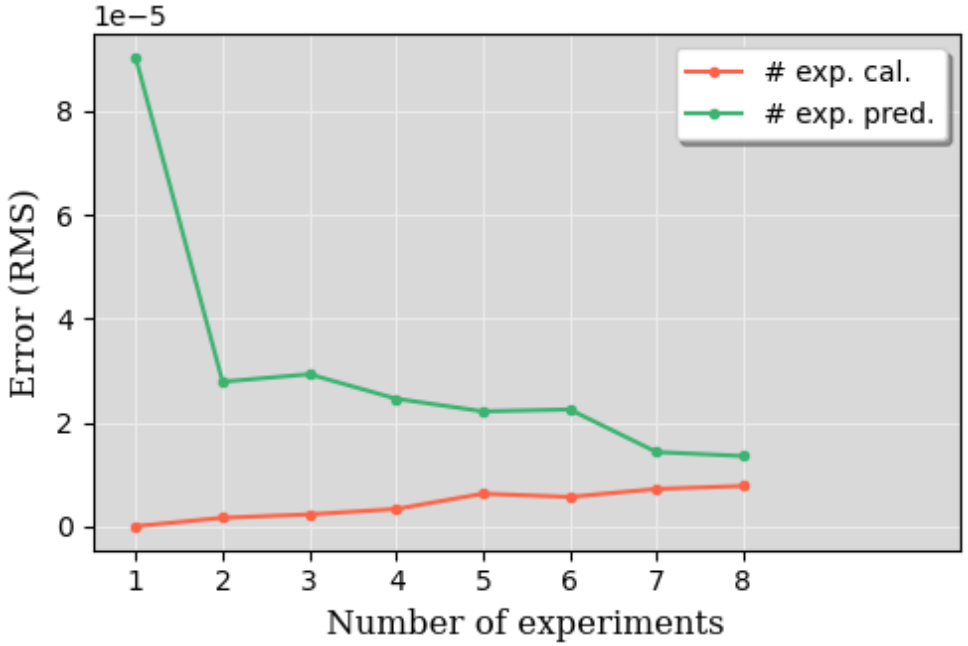
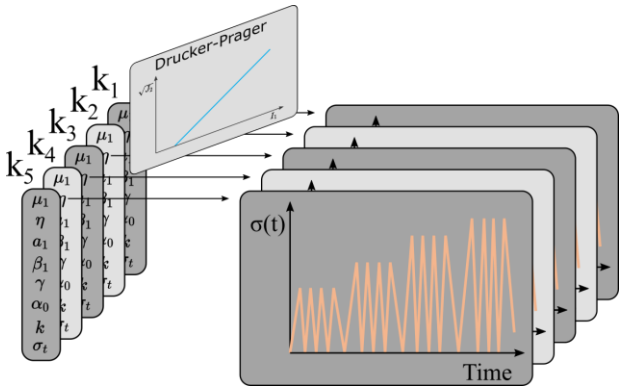


Calibration

Prediction



Test: Model unknown, parameters uncertain

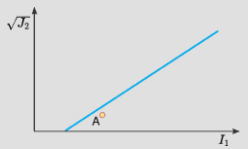


Model uncertainty: YES
Property uncertainties: YES

Calibration

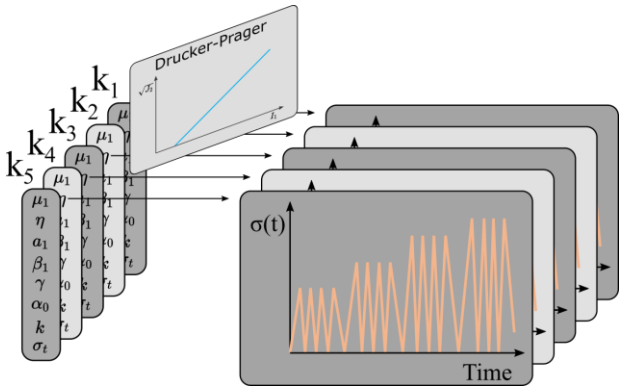
Prediction

Drucker-Prager



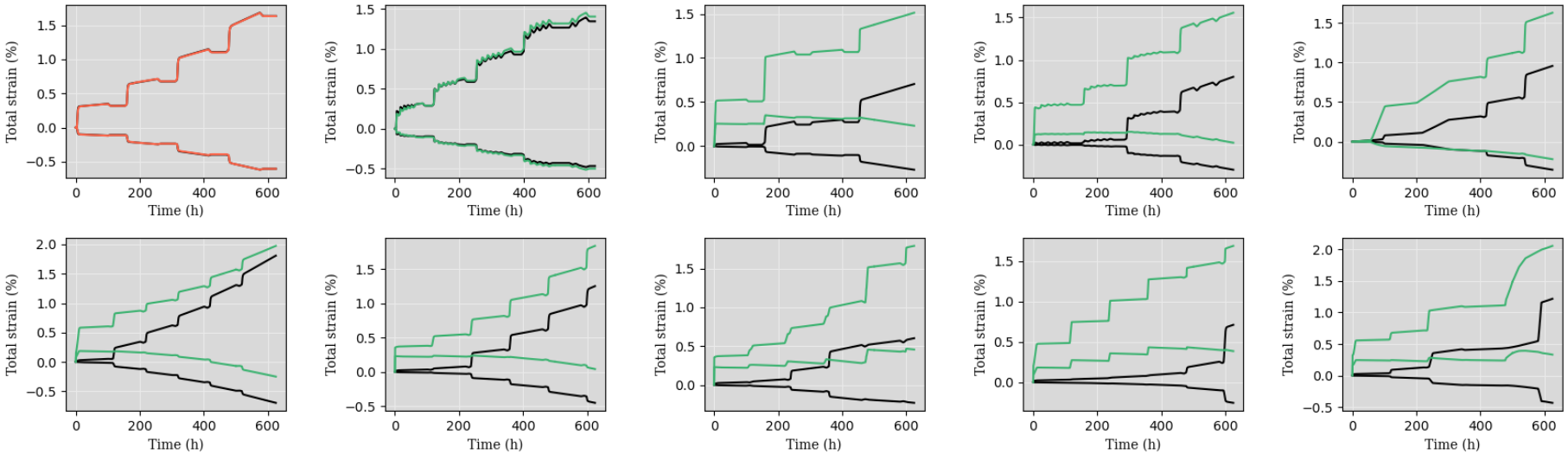
Desai

Test: Model unknown, parameters uncertain



Model uncertainty: YES

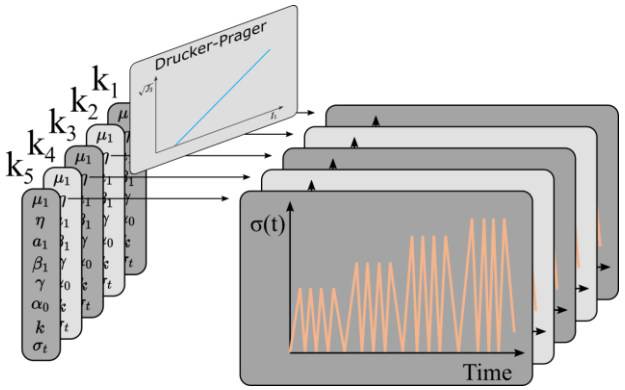
Property uncertainties: YES



Calibration

Prediction

Test: Model unknown, parameters uncertain



Model uncertainty: YES
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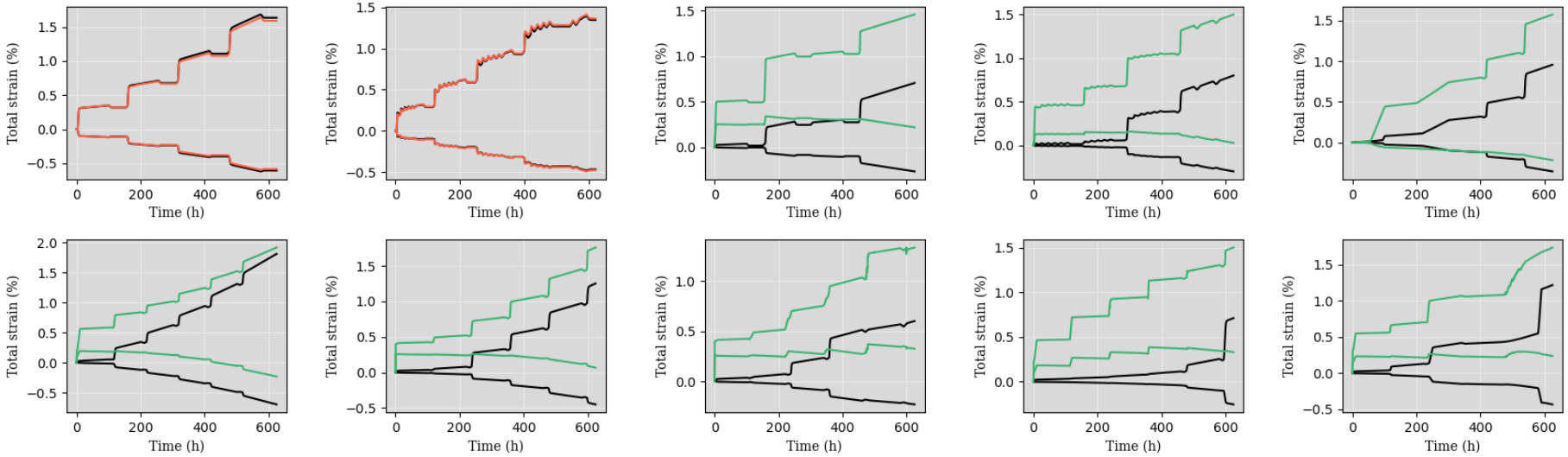

Calibration

Prediction

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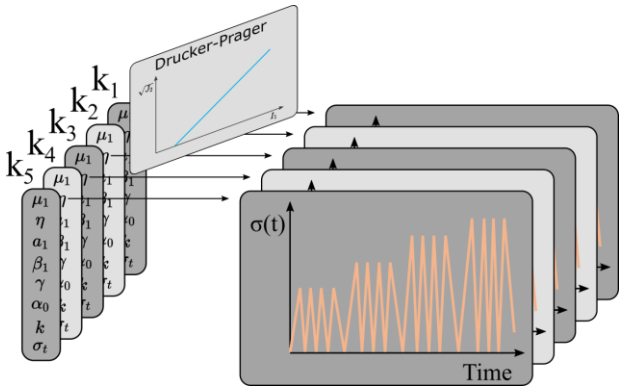
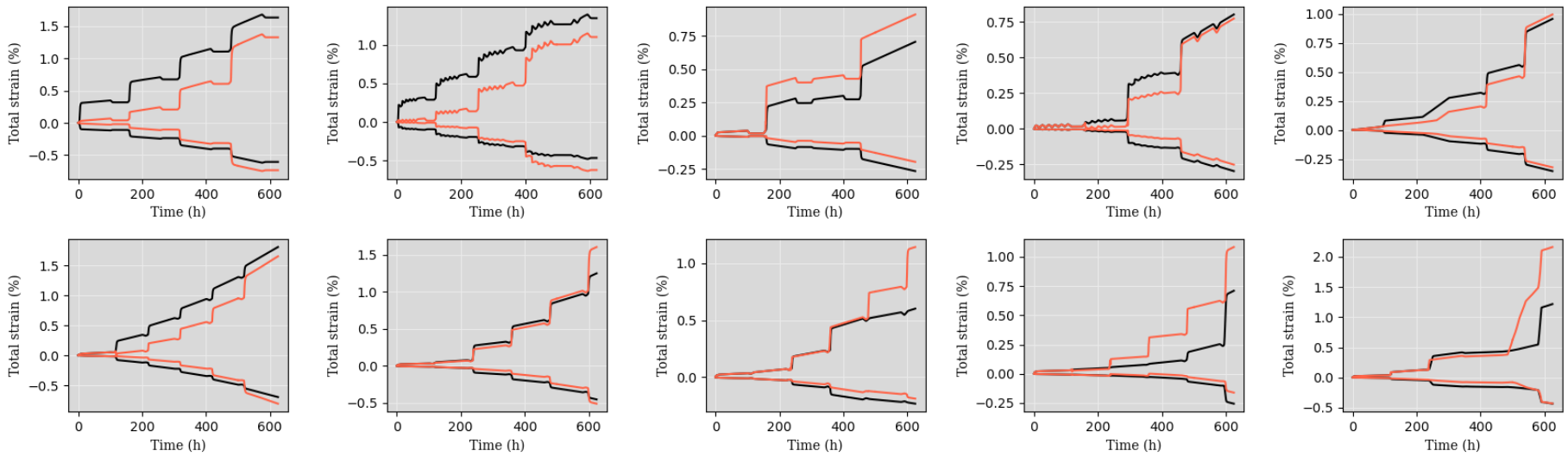


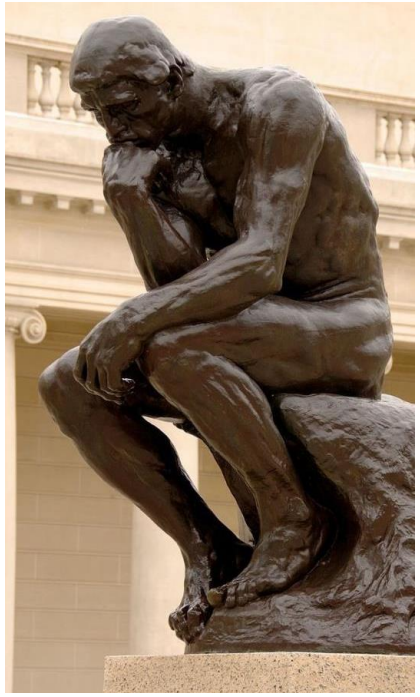
Model uncertainty: YES
Property uncertainties: YES



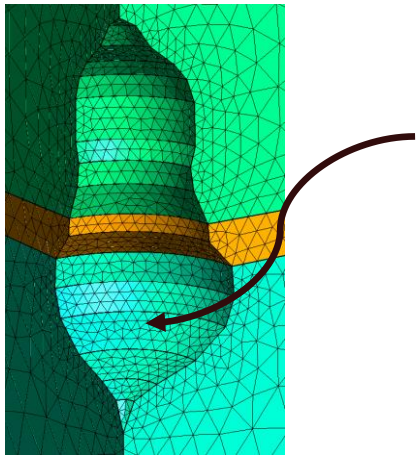
Calibration

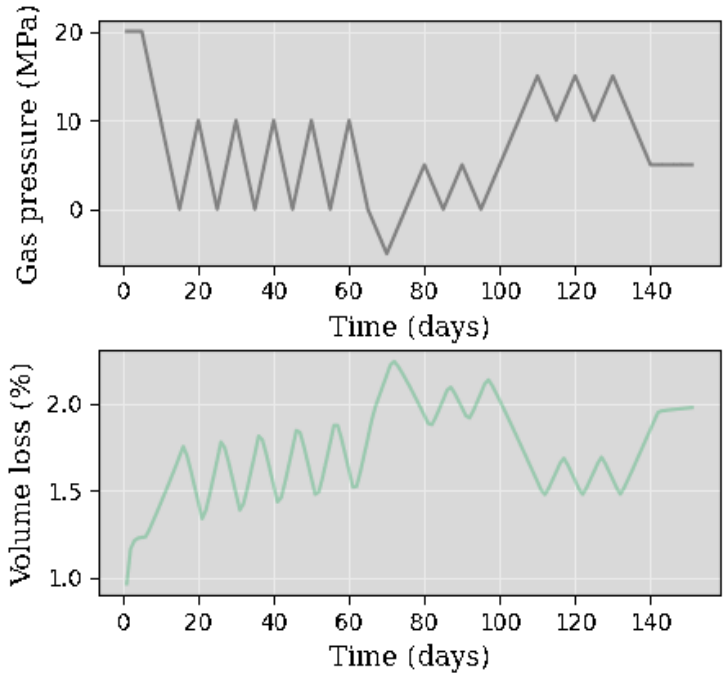
Prediction

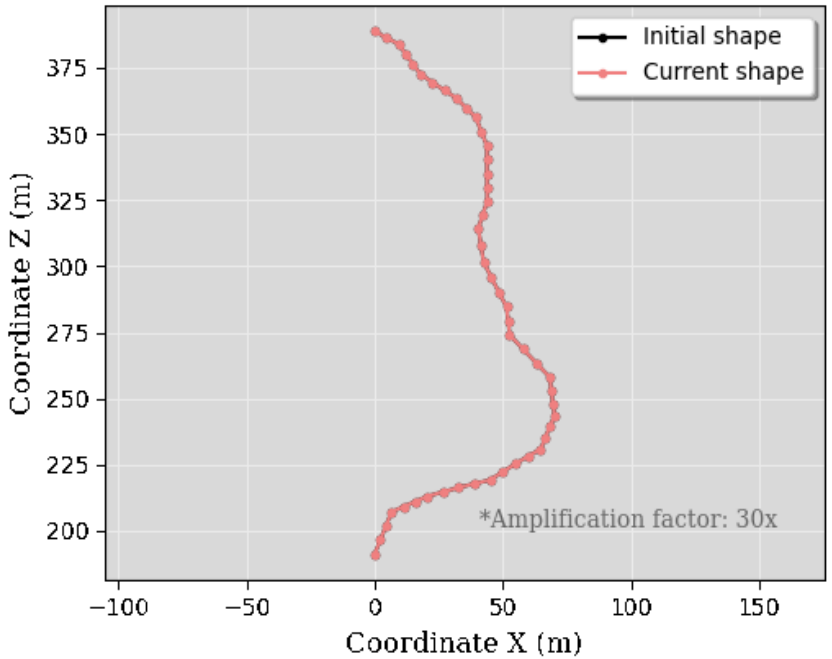
When it is impossible to match, change the model!



After calibration, perform 3D complex simulations

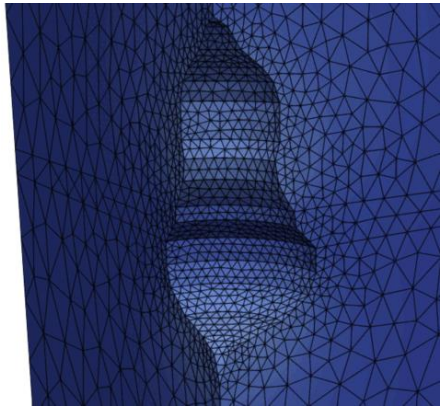






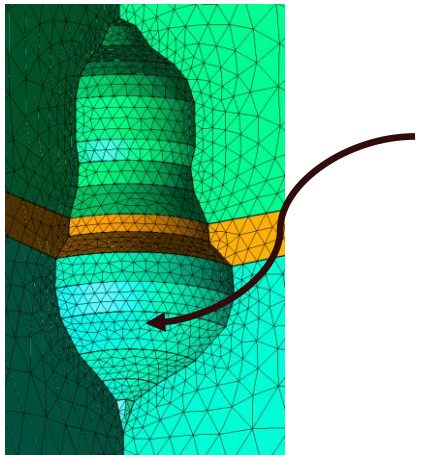
Performance analyses & closure …. with the impact of

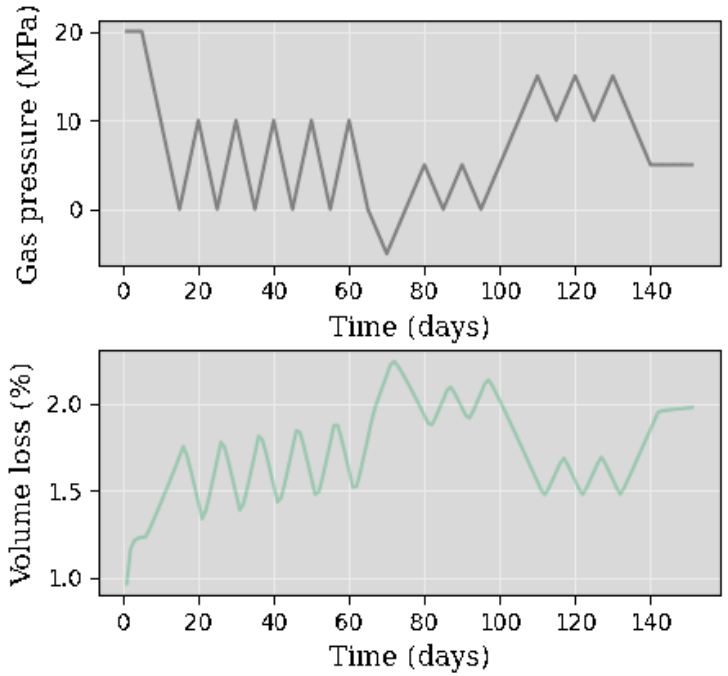
- ✓ Geometries, heterogeneities, operational cycles
- ✓ Deformation mechanisms: elastic, viscoelastic, creep, viscoplastic, thermoplastic

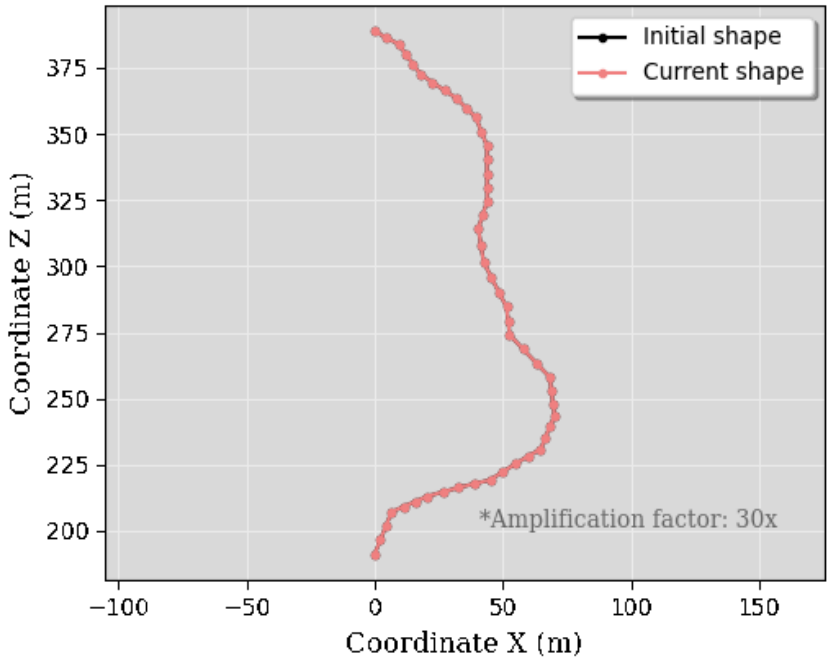


Honório & Hajibeygi, arXiv preprint arXiv:2407.18777 (2024)

After calibration, perform 3D complex simulations





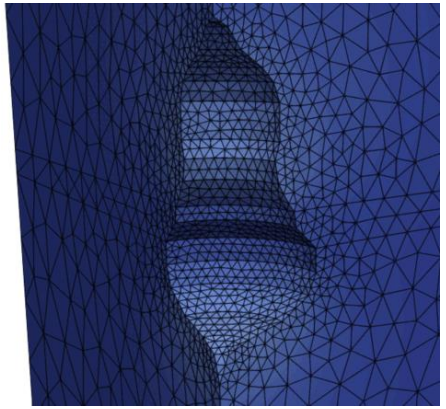


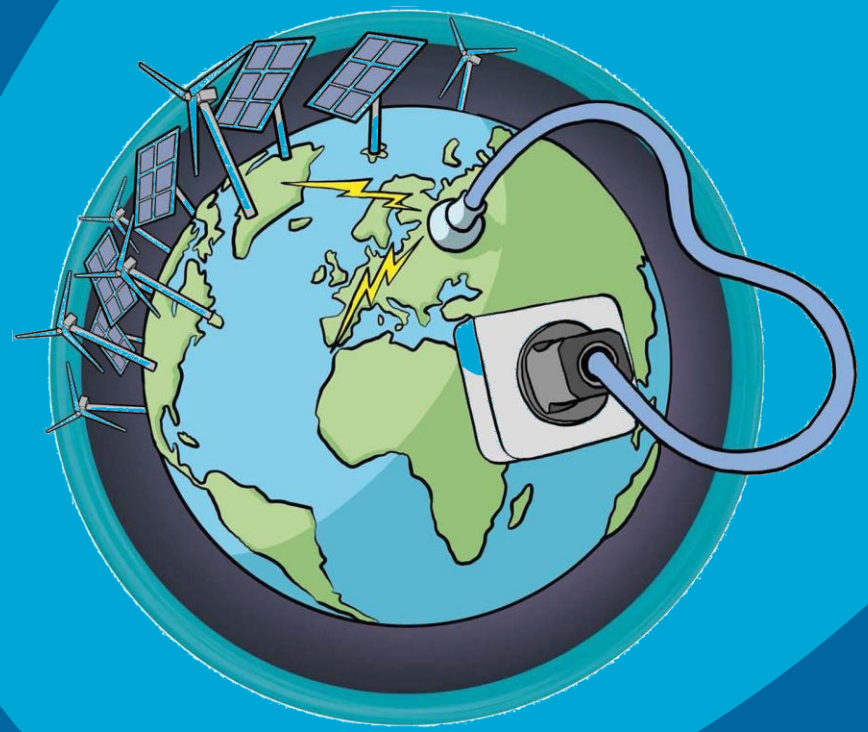
Performance analyses & closure …. with the impact of

- ✓ Geometries, heterogeneities, operational cycles
- ✓ Deformation mechanisms: elastic, viscoelastic, creep, viscoplastic, thermoplastic

Current Work: structure integrity analyses & induced seismicity risks & subsidence with including also pressure solution, damage, H2-exposure, …

Future: connect with monitoring data (or physical twins)





Thank You

Prof.dr. Hadi Hajibeygi

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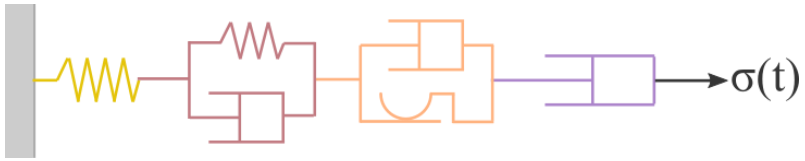
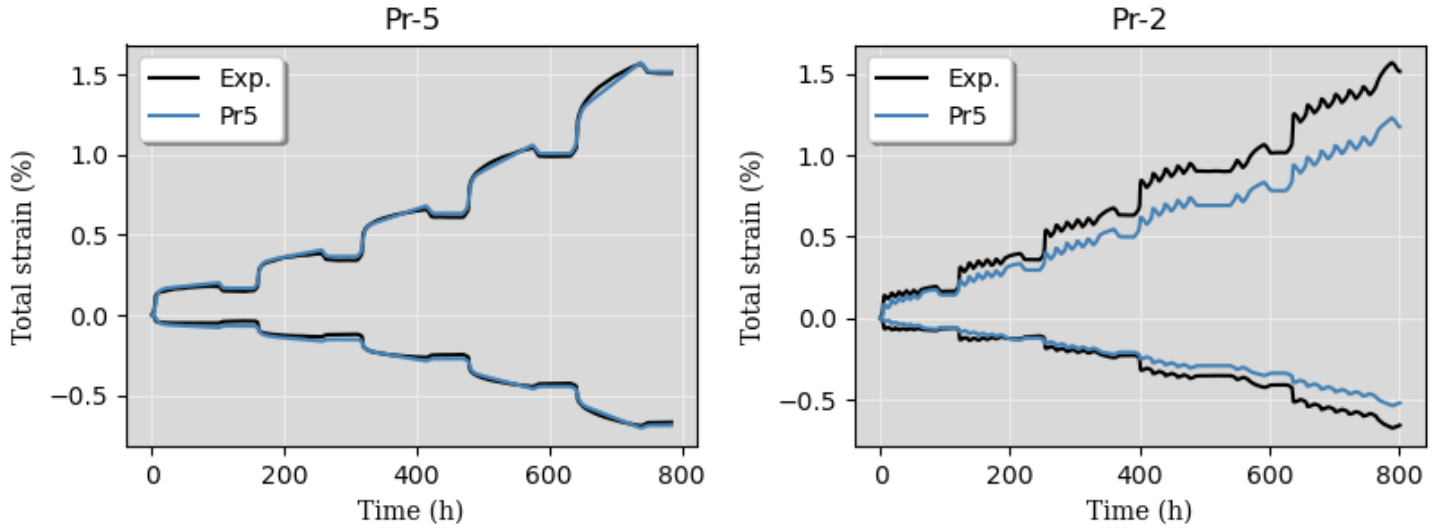
Model Selection & Parameter Calibration



Calibration →



- 2 experiments on similar samples!
- Calibrating **k** with Test1 is not predictive for Test 2! & vice versa
- How do we reliably calibrate material properties **k**?

3D Salt Cavern Simulation

Mathematical formulation

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{b}$$

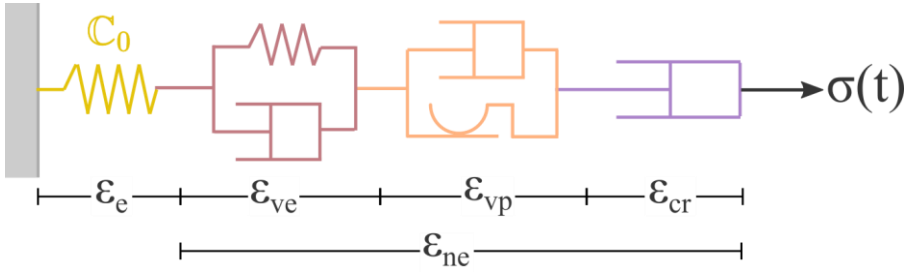
$$\boldsymbol{\sigma} = \mathbb{C}_0 : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_{ve} - \boldsymbol{\varepsilon}_{vp} - \boldsymbol{\varepsilon}_{cr}\right)$$

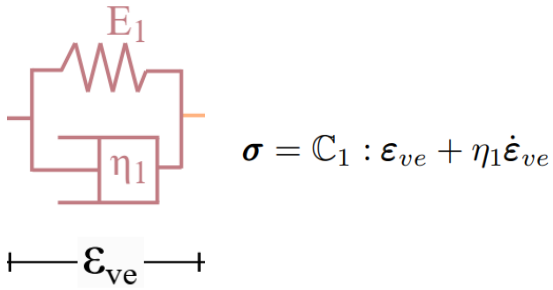
$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla \mathbf{u} + \nabla \mathbf{u}^T\right)$$

$$\boldsymbol{\varepsilon}_{ve} = \boldsymbol{\varepsilon}_{ve}\left(\boldsymbol{\sigma}\right)$$

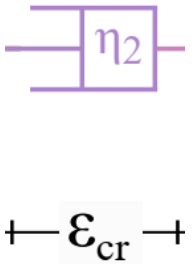
$$\boldsymbol{\varepsilon}_{vp} = \boldsymbol{\varepsilon}_{vp}\left(\boldsymbol{\sigma}, \alpha\right)$$

$$\boldsymbol{\varepsilon}_{cr} = \boldsymbol{\varepsilon}_{cr}\left(\boldsymbol{\sigma}\right)$$





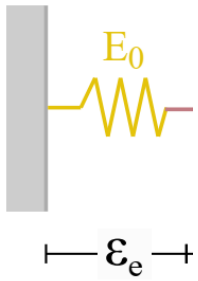
$$\boldsymbol{\sigma} = \mathbb{C}_1 : \boldsymbol{\varepsilon}_{ve} + \eta_1 \dot{\boldsymbol{\varepsilon}}_{ve}$$



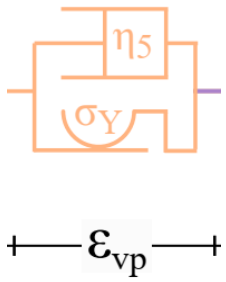
$$\mathbf{s} = \boldsymbol{\sigma} - \mathrm{tr}(\boldsymbol{\sigma})/3$$

$$q = \sqrt{\frac{3}{2}\mathbf{s} : \mathbf{s}}$$

$$\dot{\boldsymbol{\varepsilon}}_{cr} = A \exp\left(-\frac{Q}{RT}\right) q^{n-1}\mathbf{s}$$



$$\boldsymbol{\sigma} = \mathbb{C}_0 : \boldsymbol{\varepsilon}_e$$



$$\dot{\boldsymbol{\varepsilon}}_{vp} = \mu_1 \left\langle \frac{F_{vp}}{F_0} \right\rangle^{N_1} \frac{\partial F_{vp}}{\partial \boldsymbol{\sigma}}$$

$$F_{vp}(\boldsymbol{\sigma}, \alpha) = J_2 - (-\alpha I_1^{n_1} + \gamma I_1^2)\left[\exp\left(\beta_1 I_1\right) + \beta \frac{\sqrt{27} J_3}{2\sqrt{J_2^3}}\right]^m$$

$$\alpha = a_1 \left[\left(\frac{a_1}{\alpha_0}\right)^{1/\eta} + \xi\right]^{-\eta}, \quad \text{where} \quad \xi = \int_{t_0}^{t} \sqrt{\dot{\boldsymbol{\varepsilon}}_{vp} : \dot{\boldsymbol{\varepsilon}}_{vp}}\,\mathrm{dt}$$

3D Salt Cavern Simulator

Mathematical formulation

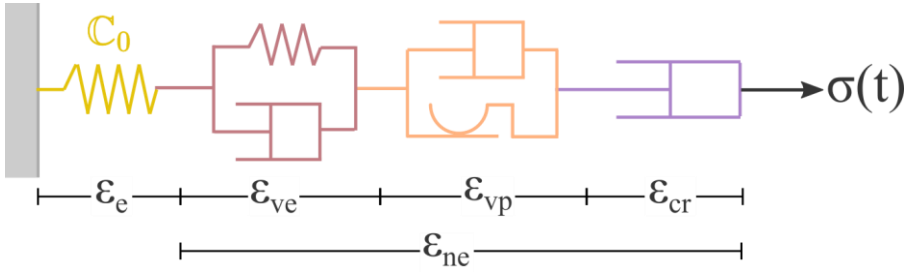


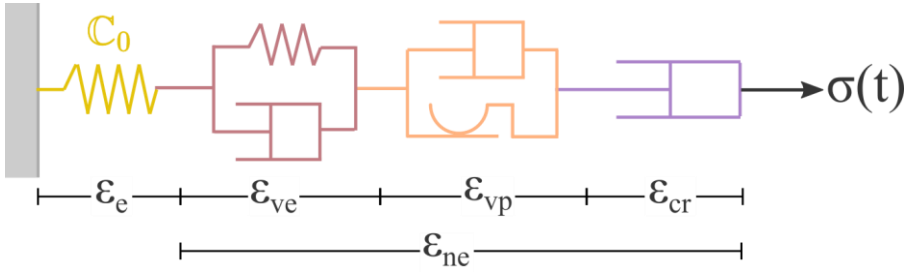
Table 1: Material parameters to be calibrated.

Group	Model	Parameters
1	Dislocation creep	A, n
2	Elastic	E_1, ν_1
	Viscoelastic	E_2, ν_2, η_2
3	Viscoplastic	μ_1, η, N_1, n_1, β, m a_1, β_1, γ, α_0, k, σ_t

Honório, et al. "A multi-step calibration strategy for reliable parameter determination of salt rock mechanics constitutive models." arXiv preprint arXiv:2403.19426 (2024).

3D Salt Cavern Simulator

Numerical formulation



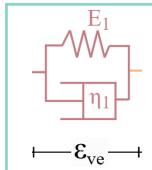
$$\nabla \cdot \mathbb{C}_T : \boldsymbol{\varepsilon}^{k+1} = \mathbf{f} + \nabla \cdot \mathbb{C}_T : \left(\bar{\boldsymbol{\varepsilon}}^k_{ne} - \phi_2 \mathbb{G}_{ne} : \boldsymbol{\sigma}^k - \phi_2 \mathbf{B}_{ne}\right)$$

$$\mathbb{C}_T = \left(\mathbb{C}_0^{-1} + \phi_2 \mathbb{G}_{ne}\right)^{-1}$$

$$\bar{\boldsymbol{\varepsilon}}^k_{ne} = \sum_{i=1}^{N_{ne}} \left(\boldsymbol{\varepsilon}^o_i + \phi_1 \dot{\boldsymbol{\varepsilon}}^o_i + \phi_2 \dot{\boldsymbol{\varepsilon}}^k_i\right)$$

$$\mathbb{G}_{ne} = \sum_{i=1}^{N_{ne}} \mathbb{G}_i$$

$$\mathbf{B}_{ne} = \sum_{i=1}^{N_{ne}} \mathbf{B}_i$$

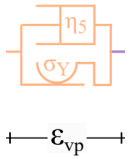


$$\mathbb{G}_{ve} = \frac{\partial \dot{\boldsymbol{\varepsilon}}_{ve}}{\partial \boldsymbol{\sigma}} = (\eta_1 \mathbb{I} + \phi_2 \mathbb{C}_1)^{-1}$$

$$\mathbf{B}_{ve} = 0$$

$$\dot{\boldsymbol{\varepsilon}}_{ve} = (\eta_1 \mathbb{I} + \phi_2 \mathbb{C}_1)^{-1} : [\boldsymbol{\sigma} - \mathbb{C}_1 : (\boldsymbol{\varepsilon}^o_{ve} + \phi_1 \dot{\boldsymbol{\varepsilon}}^o_{ve})]$$

$$\boldsymbol{\varepsilon}^{k+1}_{ve} = \boldsymbol{\varepsilon}^o_{ve} + \phi_1 \dot{\boldsymbol{\varepsilon}}^o_{ve} + \phi_2 \left(\dot{\boldsymbol{\varepsilon}}^k_{ve} + \mathbb{G}_{ve} : \delta\boldsymbol{\sigma}\right)$$



$$\mathbb{G}_{vp} = \frac{\partial \dot{\boldsymbol{\varepsilon}}_{vp}}{\partial \boldsymbol{\sigma}} - \frac{1}{h^k_{vp}} \frac{\partial \dot{\boldsymbol{\varepsilon}}_{vp}}{\partial \alpha} \frac{\partial r^k_{vp}}{\partial \boldsymbol{\sigma}}$$

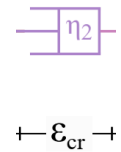
$$\mathbf{B}^k_{vp} = \frac{r^k_{vp}}{h^k_{vp}} \frac{\partial \dot{\boldsymbol{\varepsilon}}_{vp}}{\partial \alpha}$$

$$F_{vp}(\boldsymbol{\sigma}, \alpha) = J_2 - (-\alpha I_1^{n_1} + \gamma I_1^2) \left[\exp(\beta_1 I_1) + \beta \frac{\sqrt{27} J_3}{2\sqrt{J_2^3}}\right]^m$$

$$\dot{\boldsymbol{\varepsilon}}_{vp} = \mu_1 \left\langle \frac{F_{vp}}{F_0} \right\rangle^{N_1} \frac{\partial F_{vp}}{\partial \boldsymbol{\sigma}}$$

$$r^k_{vp} = \alpha^k - a_1 \left[\left(\frac{a_1}{\alpha_0}\right)^{1/\eta} + \xi^k\right]^{-\eta}, \quad \text{where} \quad \xi^k = \int_{t_0}^{t} \sqrt{\dot{\boldsymbol{\varepsilon}}^k_{vp} : \dot{\boldsymbol{\varepsilon}}^k_{vp}} \mathrm{d}t$$

$$h^k_{vp} = \frac{\partial r^k_{vp}}{\partial \alpha}$$



$$\mathbb{G}_{cr} = \frac{\partial \dot{\boldsymbol{\varepsilon}}_{cr}}{\partial \boldsymbol{\sigma}}$$

$$\mathbf{B}_{cr} = 0$$

$$\mathbf{s} = \boldsymbol{\sigma} - \mathrm{tr}(\boldsymbol{\sigma})/3$$

$$q = \sqrt{\frac{3}{2} \mathbf{s} : \mathbf{s}}$$

$$\dot{\boldsymbol{\varepsilon}}_{cr} = A \exp\left(-\frac{Q}{RT}\right) q^{n-1} \mathbf{s}$$

Honório, et al. "A multi-step calibration strategy for reliable parameter determination of salt rock mechanics constitutive models." arXiv preprint arXiv:2403.19426 (2024).