

# A temperature-dependent constitutive model for argillaceous hard soils - weak rocks

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## 1 Introduction

## 2 Implementation of thermal effects

- Volumetric yield function
- Temperature dependence of the **deviatoric** yield surface
- Temperature dependence of the **volumetric** yield surface
- Additional convergence checks

## 3 Coupled THM BVP simulation

## 4 Conclusions

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- The aim is to remove the residues from the human environment and to ensure release rates of radionuclides below allowable limits.

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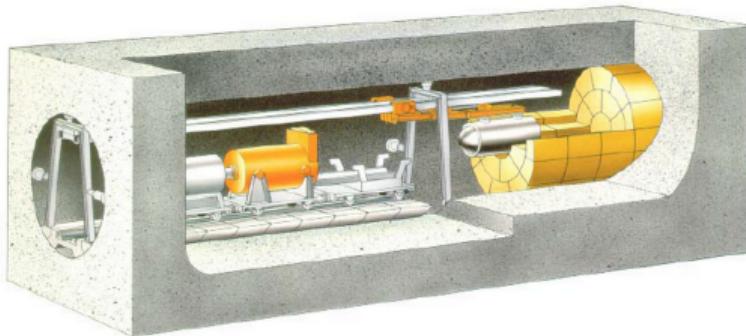
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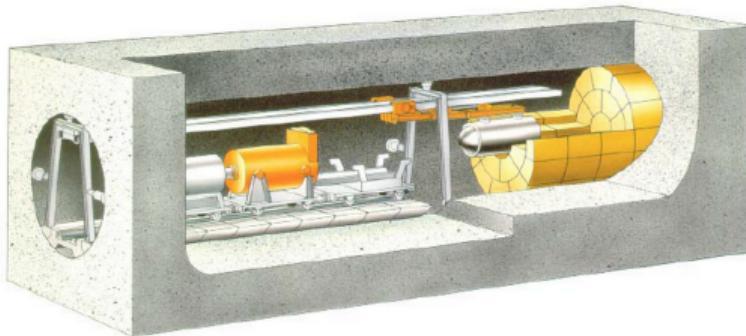


(Gens, 2004)

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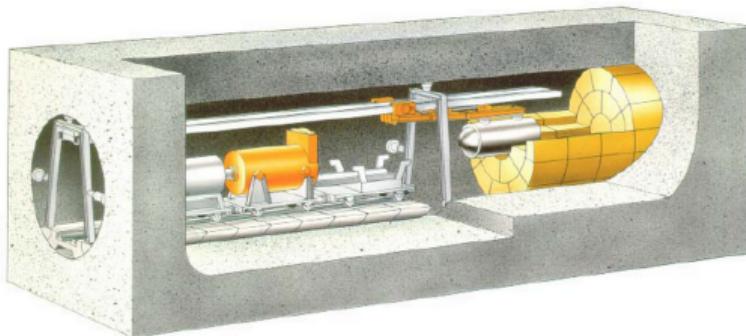
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- Possible geological barriers:
  - Salt rocks
  - Argillaceous rocks
  - Limestones
  - Granite rock
  - Basalt rock
  - Volcanic tuff

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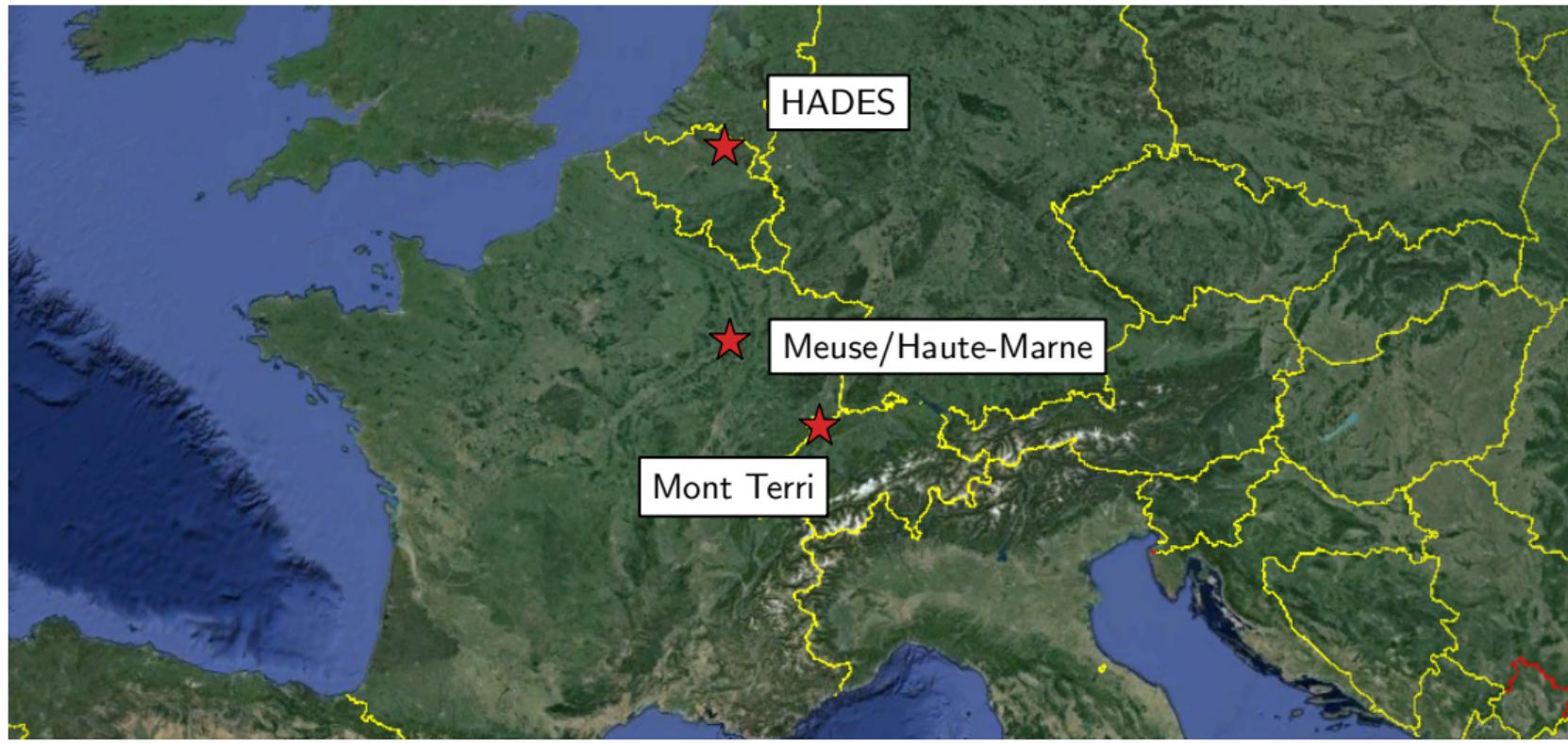
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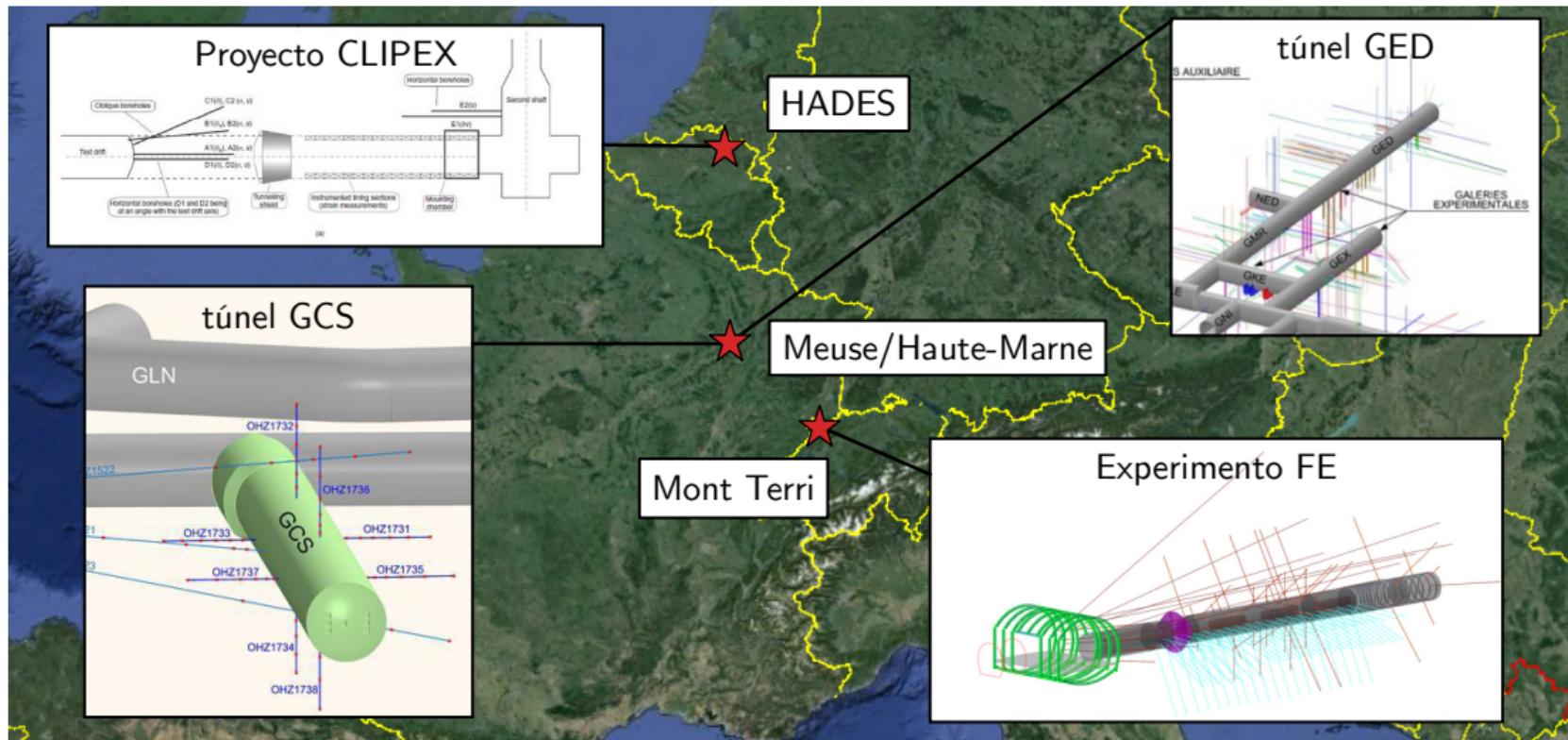
# Introduction



# Introduction



# Introduction



# Introduction - Constitutive model for the host rock

## Strain decomposition

$$d\epsilon = d\epsilon^e + d\epsilon^{vp} + d\epsilon^c$$

## Elastic behaviour (cross-anisotropy)

$$\begin{aligned} d\sigma &= \hat{\mathbf{D}}^e d\epsilon^e \\ \hat{\mathbf{D}}^e &= \mathbf{T}^T \mathbf{D}^e \mathbf{T} \end{aligned}$$

## Yield criterion

$$f = \sqrt{\frac{J_2}{f_d(\theta)} + (c^* + p_t \tan \phi^*)^2} - (c^* + p' \tan \phi^*)$$

$$f_d(\theta) = \alpha_d (1 + B_d \sin 3\theta)^n$$

## Strength anisotropy

$$\begin{aligned} p_t &= \Omega(\delta)p_{t0} \\ \Omega &= \frac{A e^{(\delta_m - \delta)n}}{\left[1 + e^{(\delta_m - \delta)n}\right]^2} + \frac{B}{1 + e^{(\delta_m - \delta)n}} + C \end{aligned}$$

## Softening laws

$$\tan \phi^* = \tan \phi_{peak}^* - \left( \tan \phi_{peak}^* - \tan \phi_{res}^* \right) \left[ 1 - e^{-b_{res}(\epsilon_{eq}^p)} \right]$$

$$c_0^* = \left( c_{0\text{ peak}}^* - c_{0\text{ post}}^* \right) e^{-b_{post}(\epsilon_{eq}^p)} + c_{0\text{ post}}^* e^{-b_{res}(\epsilon_{eq}^p)}$$

$$p_{t0} = \left( p_{t0\text{ peak}} - p_{t0\text{ post}} \right) e^{-b_{post}(\epsilon_{eq}^p)} + p_{t0\text{ post}} e^{-b_{res}(\epsilon_{eq}^p)}$$

$$\epsilon_{eq}^p = (\epsilon^p : \epsilon^p)^{1/2} \quad \epsilon^p = \epsilon^{vp} + \epsilon^c$$

## Flow rule

$$\frac{\partial G}{\partial \sigma'} = \omega \frac{\partial F}{\partial p} \frac{\partial p}{\partial \sigma'} + \frac{\partial F}{\partial J_2} \frac{\partial J_2}{\partial \sigma'} + \frac{\partial F}{\partial \theta} \frac{\partial \theta}{\partial \sigma'}$$

## Visco-plasticity

$$\begin{aligned} d\epsilon^{vp} &= \frac{\langle \Phi(F) \rangle}{\eta} \frac{\partial G}{\partial \sigma'} dt \\ \Phi(F) &= \left( \frac{F}{p_{atm}} \right)^N \end{aligned}$$

## Creep deformations

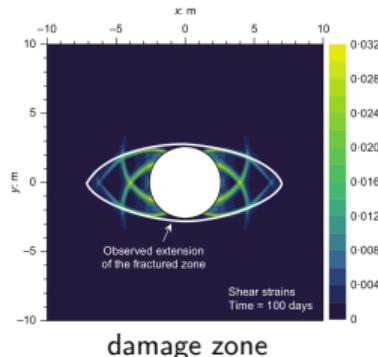
$$\begin{aligned} d\epsilon^c &= \dot{\epsilon}^c dt \\ \dot{\epsilon}^c &= \begin{cases} \mathbf{0} & \text{if } \epsilon_{eq}^p \leq \epsilon_{thr} \\ \gamma e^{(-m\epsilon_{eq}^c)} \left( \mathbf{s} + \mu p' \mathbf{I} \right) & \text{if } \epsilon_{eq}^p > \epsilon_{thr} \end{cases} \\ \epsilon_{eq}^c &= (\epsilon^c : \epsilon^c)^{1/2} \end{aligned}$$

## Nonlocal regularisation

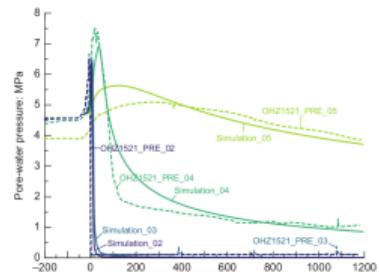
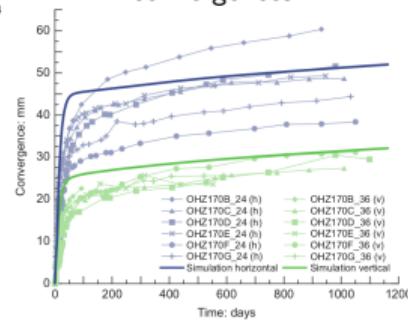
$$\begin{aligned} \bar{\epsilon}_{eq}^p(\mathbf{x}) &= \int_V w(\mathbf{x}, \xi) \epsilon_{eq}^p(\xi) d\xi \\ w(\mathbf{x}, \xi) &= \frac{w_0(\|\mathbf{x} - \xi\|)}{\int_V w_0(\|\mathbf{x} - \zeta\|) d\zeta} \\ w_0 &= \frac{\|\mathbf{x} - \xi\|}{l_s} e^{-\left( \frac{\|\mathbf{x} - \xi\|}{l_s} \right)^2} \end{aligned}$$

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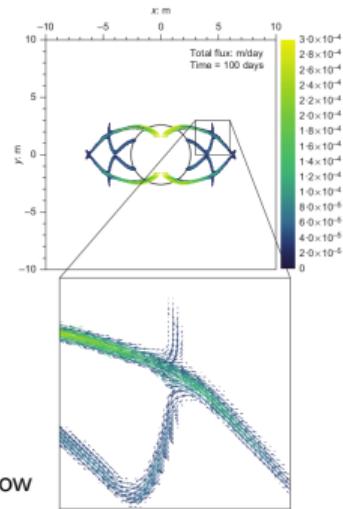
- *Hydromechanical behaviour of excavations*



horizontal and vertical convergences



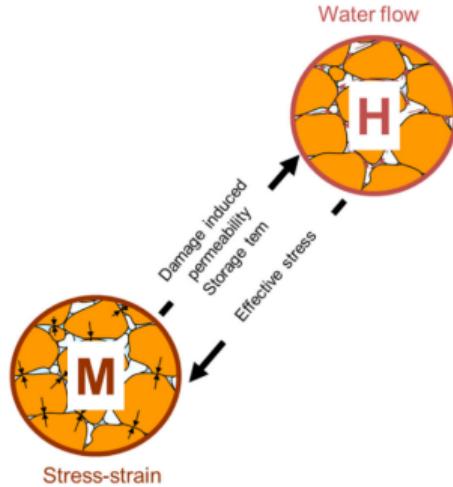
water pressures



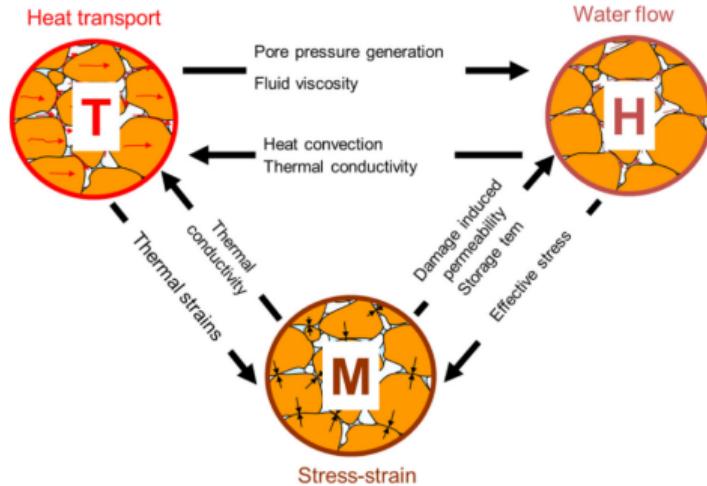
localised water flow

(Mánica et al., 2022)

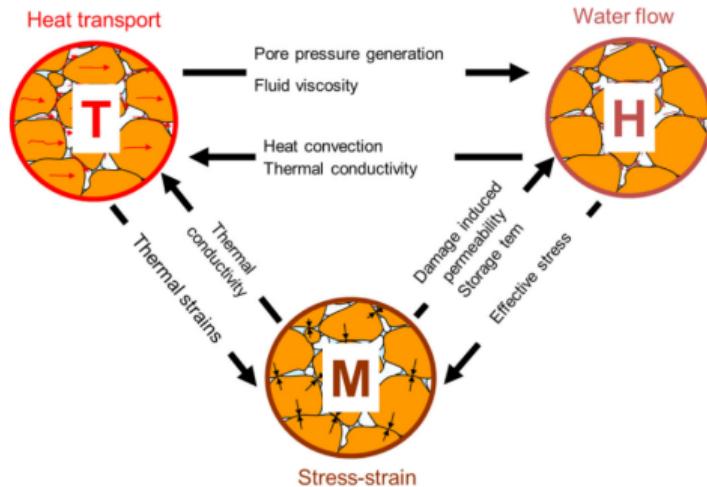
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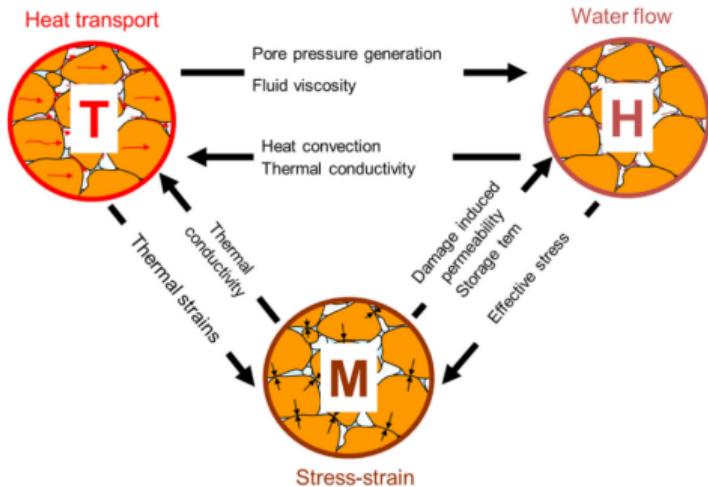
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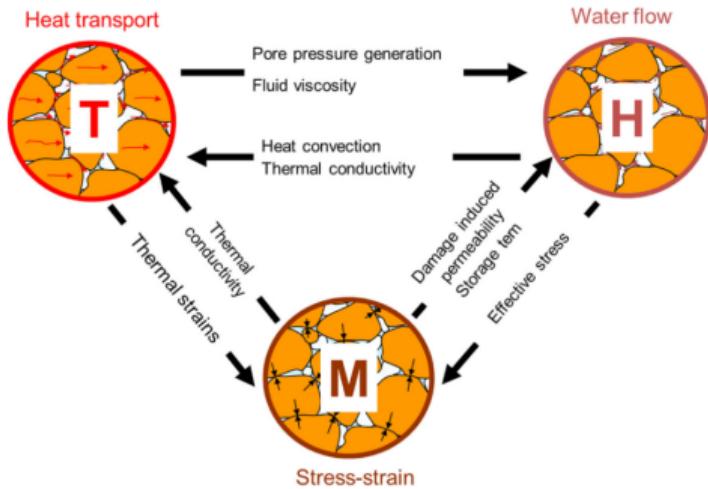
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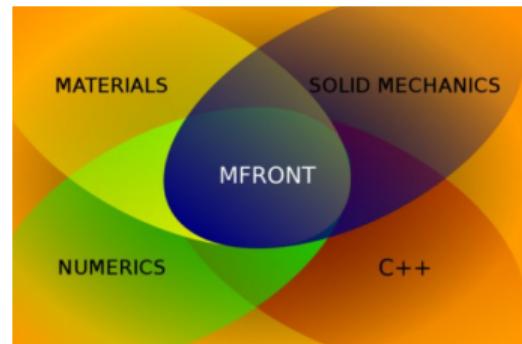
- The main objective is to incorporate thermal effects into the constitutive description of the host rock.



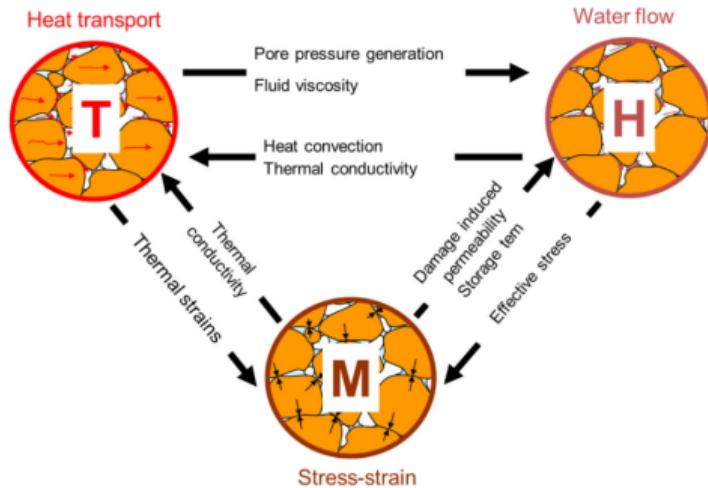
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- Implementation of the constitutive model through **MFront**.



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- Implementation of the constitutive model through **MFront**.
- To be used in coupled THM simulations using the finite element code **OpenGeoSys**



**OpenGeoSys**  
OPEN-SOURCE MULTI-PHYSICS

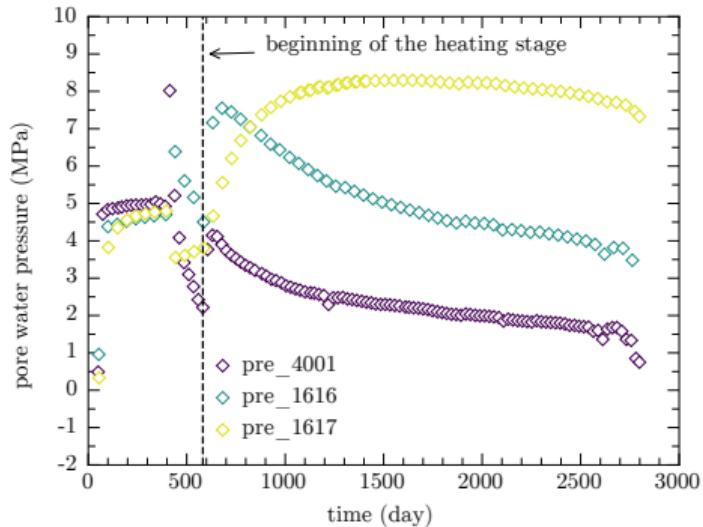
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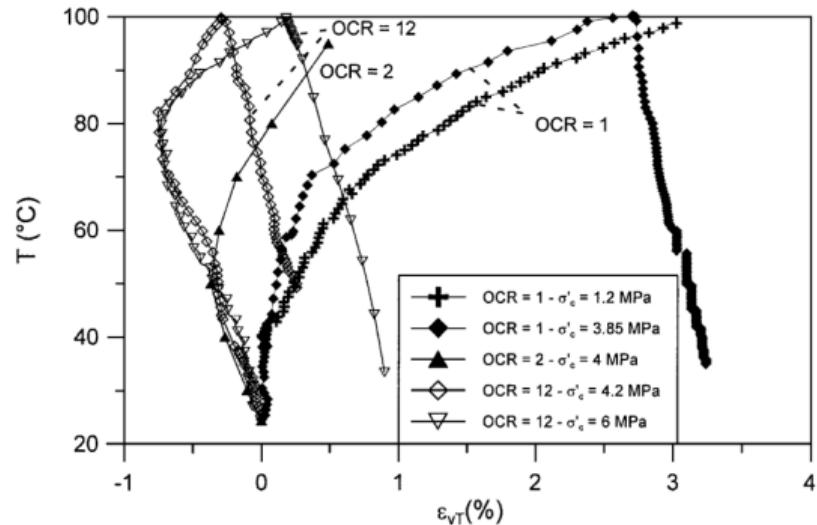


COx claystone (Bumbieler et al., 2021)

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## *Thermal behaviour of argillaceous hard soils - weak rocks*

- Thermal pressurisation
- **Thermal volume changes**

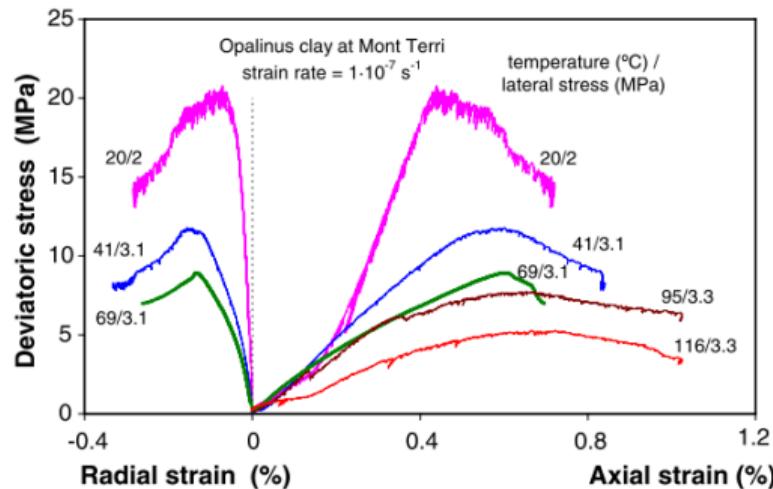


Boom clay (Sultan et al., 2002)

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## *Thermal behaviour of argillaceous hard soils - weak rocks*

- Thermal pressurisation
- Thermal volume changes
- Variation of mechanical properties



Opalinus clay (Zhang et al., 2007)

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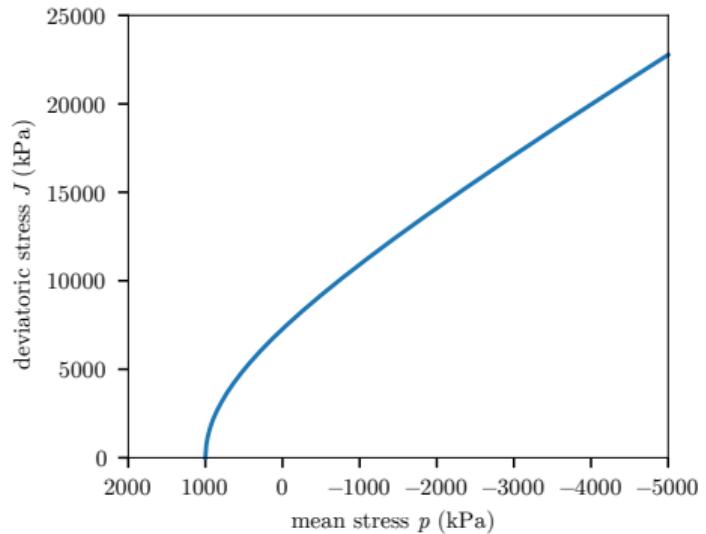
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# Volumetric yield function

- Originally only a deviatoric yield mechanism was considered:

$$f_1 = \sqrt{\frac{J_2}{f_d(\theta)} + (c^* + p_t \tan \phi^*)^2} - (c^* + p' \tan \phi^*)$$



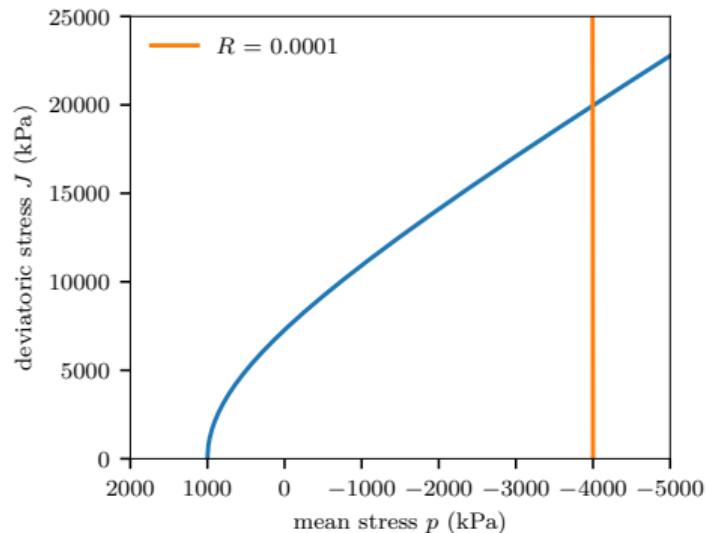
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$$f_2 = R^2 J^2 + p_c - p'$$



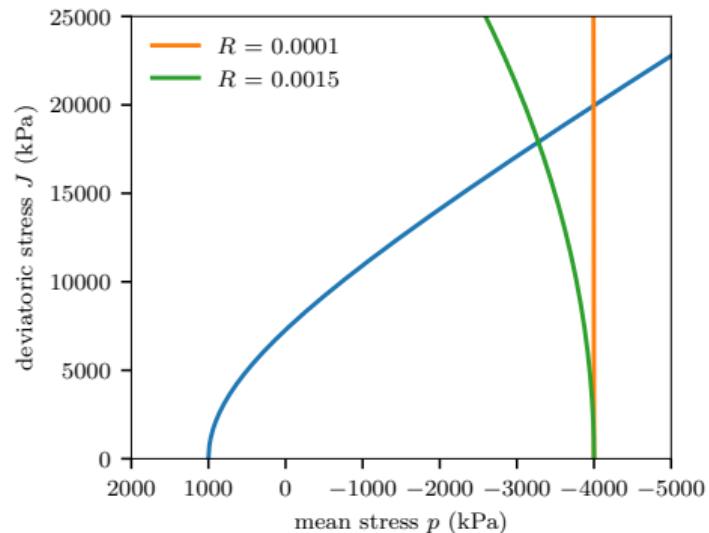
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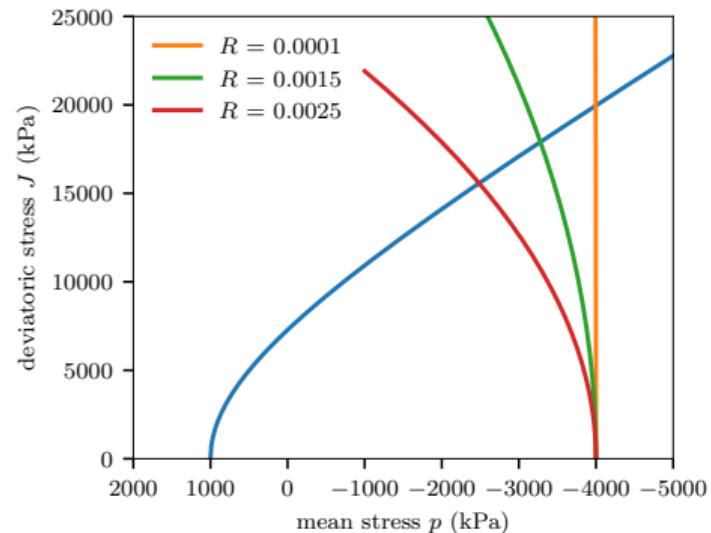
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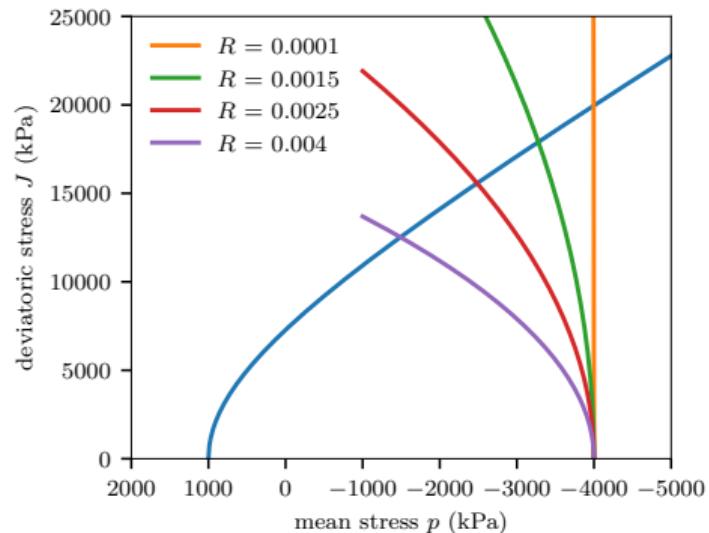
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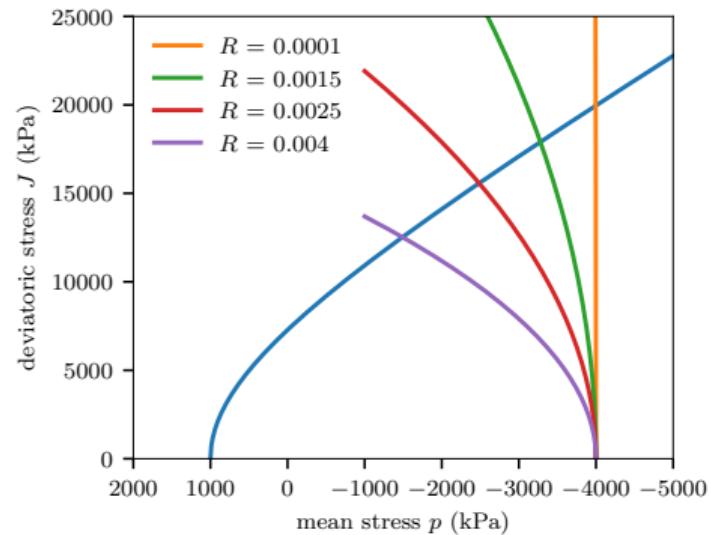
- Multi-surface plasticity framework:

$$\mathcal{E} = \{\boldsymbol{\sigma} \mid F_i(\boldsymbol{\sigma}, \alpha_i) < 0, i = 1, \dots, n\}$$

$$F_i(\boldsymbol{\sigma}, \alpha_i) = 0$$

$$\Delta \boldsymbol{\epsilon}^p = \sum_{i=1}^n \Delta \lambda_i \frac{\partial g_i}{\partial \boldsymbol{\sigma}}$$

$$F_i \leq 0, \quad \Delta \lambda_i \geq 0, \quad F_i \Delta \lambda_i = 0$$



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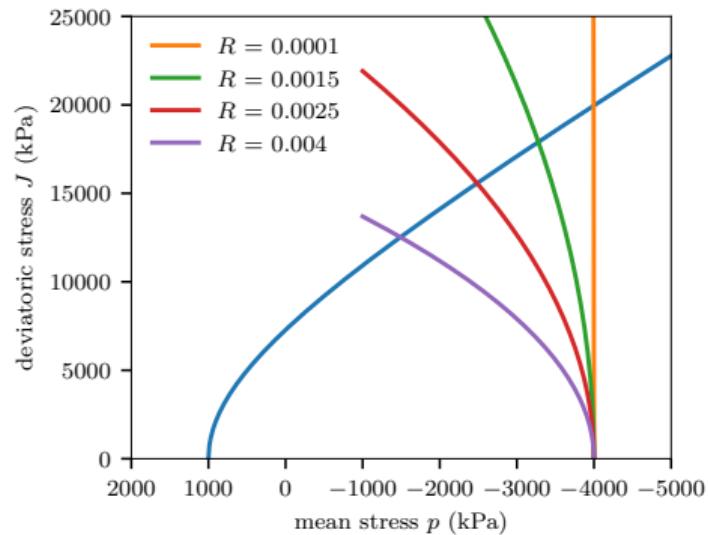
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$$F_i \leq 0, \quad \Delta \lambda_i \geq 0, \quad F_i \Delta \lambda_i = 0$$



- Linear hardening law:

$$\frac{\partial p_c}{\partial \epsilon_v^p} = \frac{K^{ep} K^e}{K^{ep} - K^e}$$

# Volumetric yield function

## *System of equations*

Activation only of the **deviatoric** yield surface.

```
feel      += dlambda*d_g_d_sig + dt*epsc_rate;
flambda  = (f - p_atm*pow(dlambda*eta_pz/dt, (1.0/N_pz)))/D(0,0);
fepsp    = depsp - dlambda*d_g_d_sig - dt*epsc_rate;
fepsc    = depsc - dt*epsc_rate;
```

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fepsp    = depsp - dlambda*d_g_d_sig - dt*epsc_rate;
fepsc    = depsc - dt*epsc_rate;
```

Activation only of the **volumetric** yield surface.

```
feel      += dlambda2*d_f2_d_sig + dt*epsc_rate;
fpc       = dpc + (K_ep*K_ave)/(K_ep-K_ave)*dlambda2*d_f2_d_p +
            (K_ep*K_ave)/(K_ep-K_ave)*(idl(dt*epsc_rate));
flambda2 = (f2 - p_atm*pow(dlambda2*eta_pz/dt, (1.0/N_pz)))/D(0,0);
fepsp    = depsp - dlambda2*d_f2_d_sig - dt*epsc_rate;
fepsc    = depsc - dt*epsc_rate;
```

# Volumetric yield function

## System of equations

Activation of both the **deviatoric** and **volumetric** yield surfaces.

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feel      += dlambda*d_g_d_sig + dt*epsc_rate + dlambda2*d_f2_d_sig;
flambda   = (f - p_atm*pow(dlambda*eta_pz/dt, (1.0/N_pz)))/D(0,0);
flambda2  = (f2 - p_atm*pow(dlambda2*eta_pz/dt, (1.0/N_pz)))/D(0,0);
fepsp     = depsp - dlambda*d_g_d_sig - dlambda2*d_f2_d_sig - dt*epsc_rate;
fepsc     = depsc - dt*epsc_rate;
fpc       = dpc + (K_ep*K_ave)/(K_ep-K_ave)*dlambda2*d_f2_d_p +
            (K_ep*K_ave)/(K_ep-K_ave)*(id|(dt*epsc_rate));
```

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## System of equations

Activation of both the **deviatoric** and **volumetric** yield surfaces.

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feel      += dlambda*d_g_d_sig + dt*epsc_rate + dlambda2*d_f2_d_sig;
flambda   = (f - p_atm*pow(dlambda*eta_pz/dt, (1.0/N_pz)))/D(0,0);
flambda2  = (f2 - p_atm*pow(dlambda2*eta_pz/dt, (1.0/N_pz)))/D(0,0);
fepsp     = depsp - dlambda*d_g_d_sig - dlambda2*d_f2_d_sig - dt*epsc_rate;
fepsc     = depsc - dt*epsc_rate;
fpc       = dpc + (K_ep*K_ave)/(K_ep-K_ave)*dlambda2*d_f2_d_p +
            (K_ep*K_ave)/(K_ep-K_ave)*(id|(dt*epsc_rate));
```

None of the yield surfaces are active but **creep** have been activated::

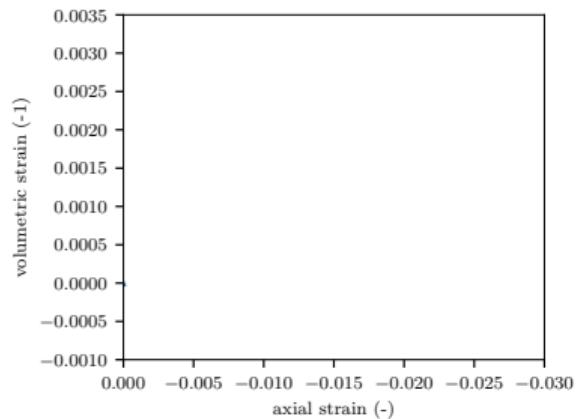
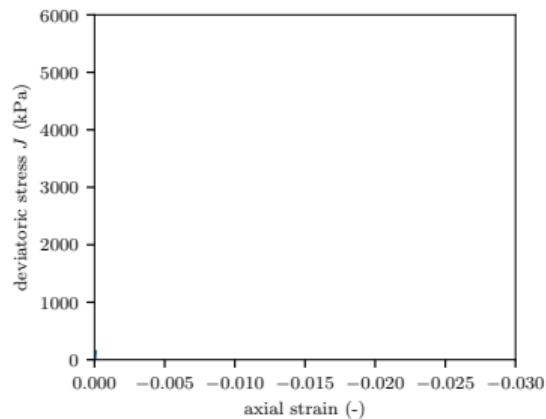
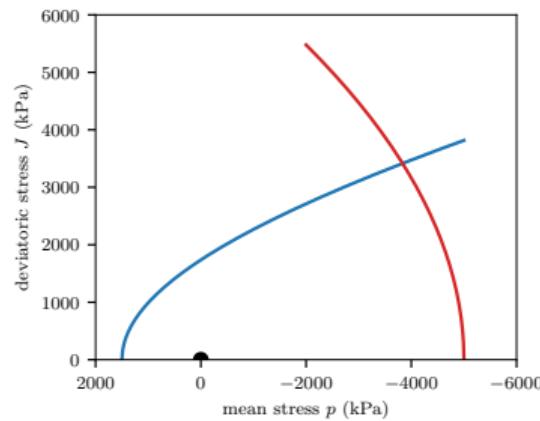
```
feel      += dt*epsc_rate;
fepsp    = depsp - dt*epsc_rate;;
fepsc    = depsc - dt*epsc_rate;
```

# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*

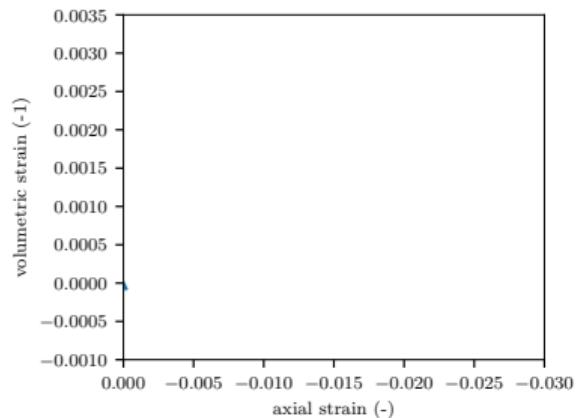
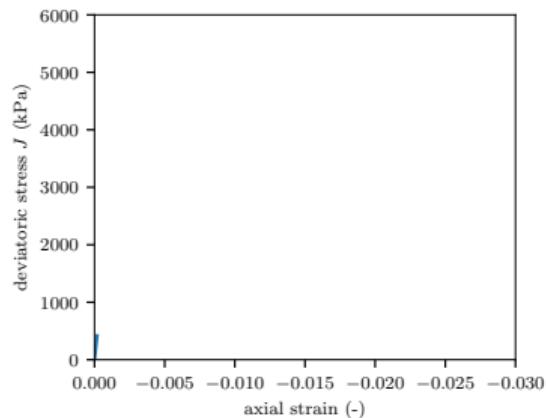
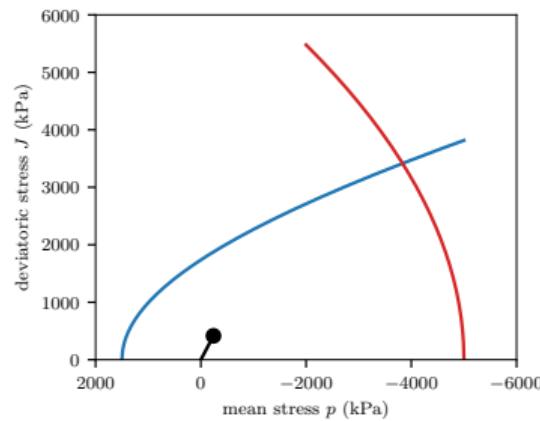
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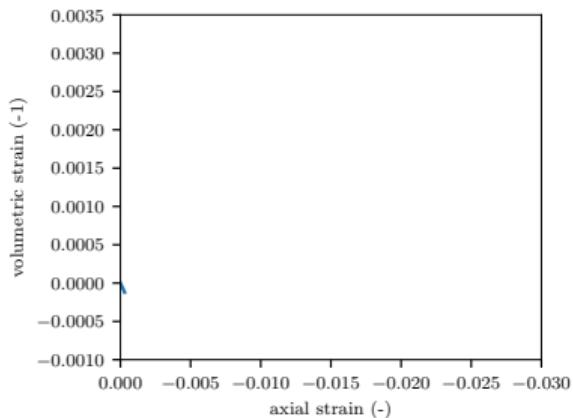
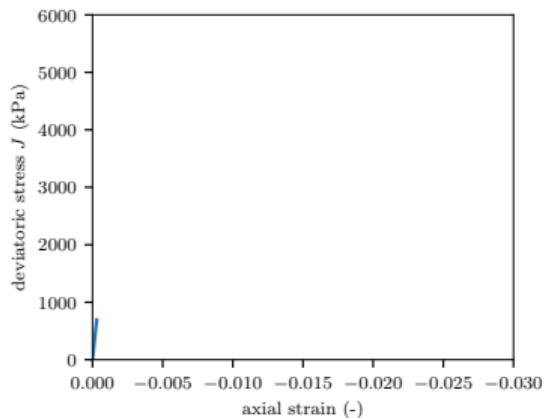
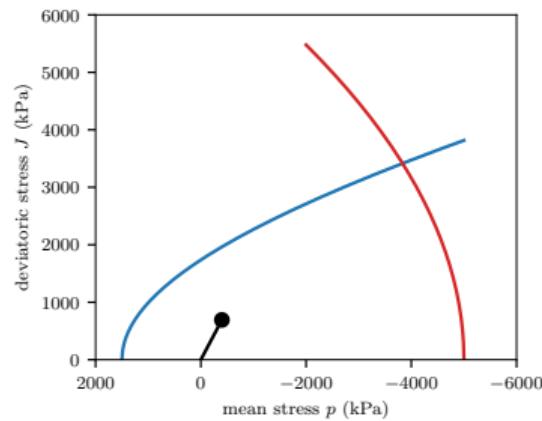
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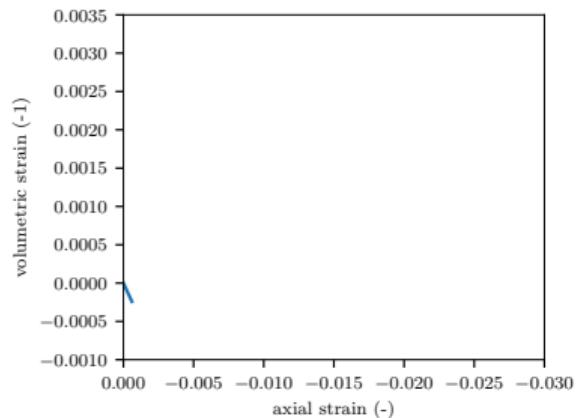
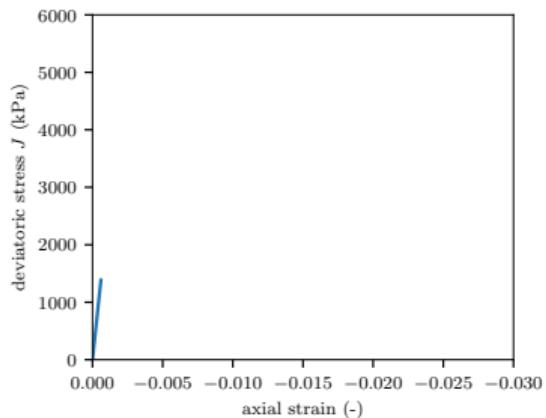
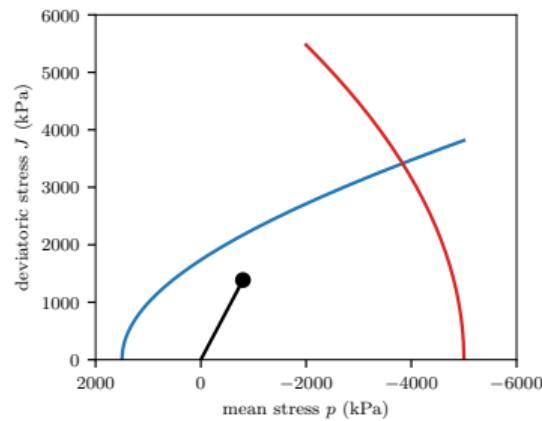
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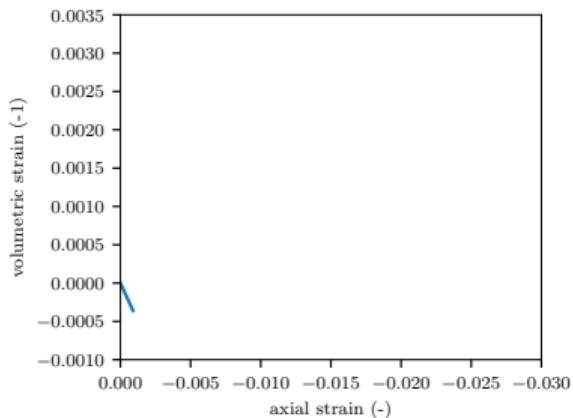
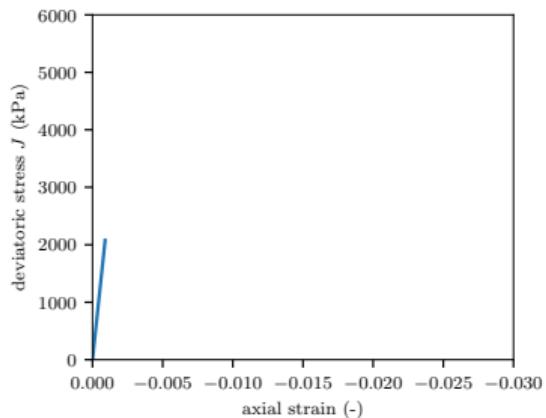
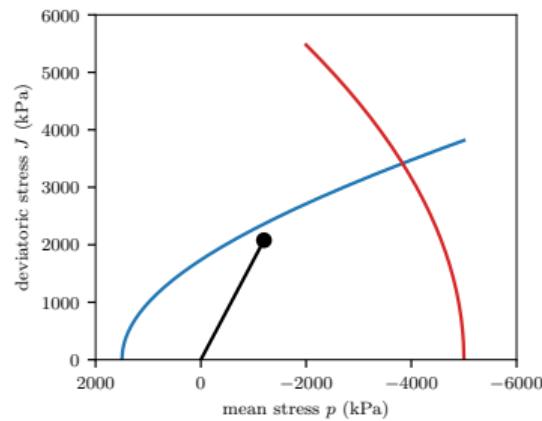
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



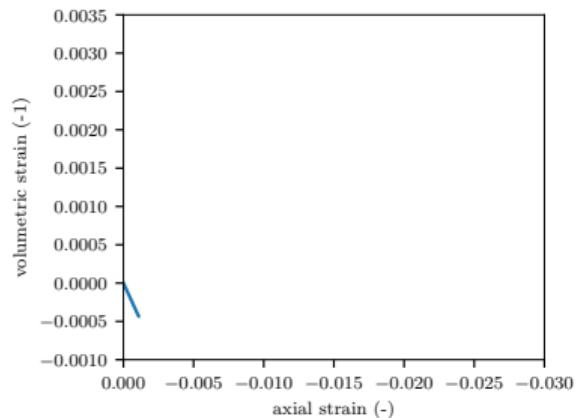
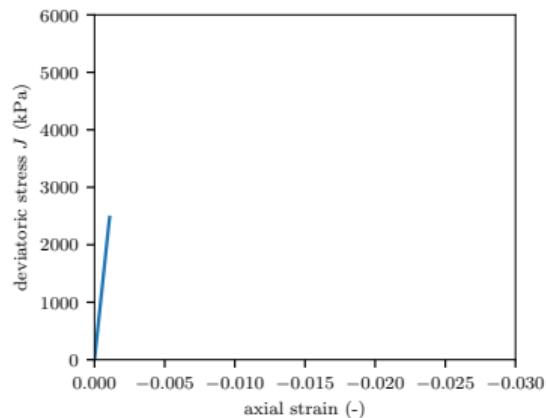
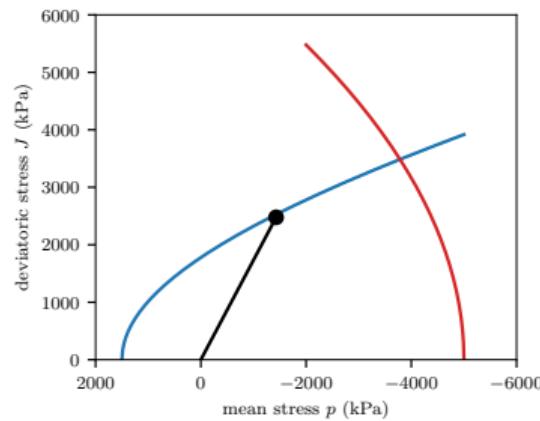
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



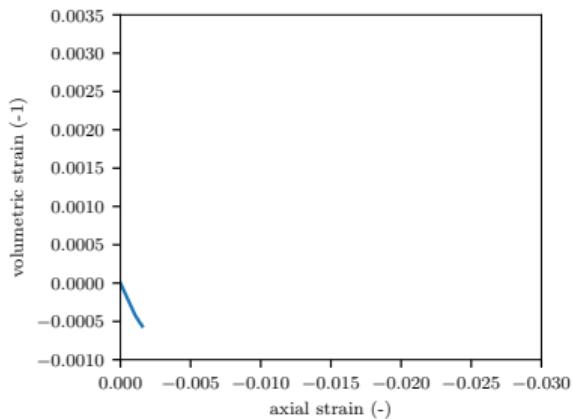
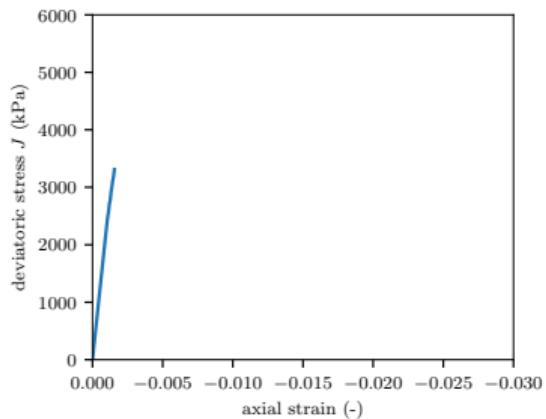
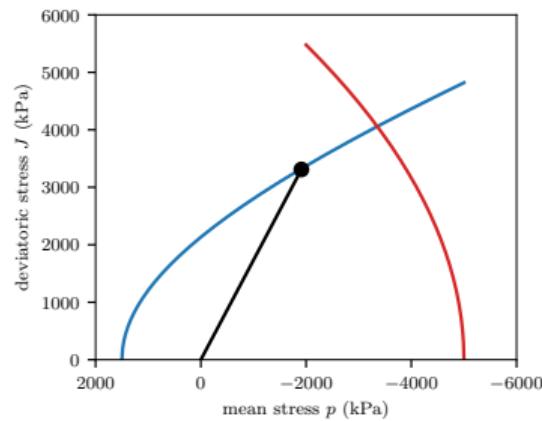
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



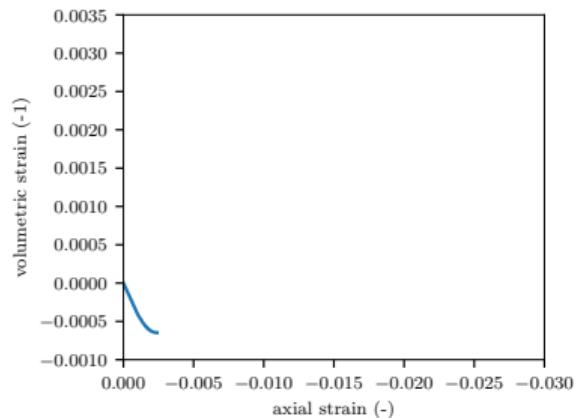
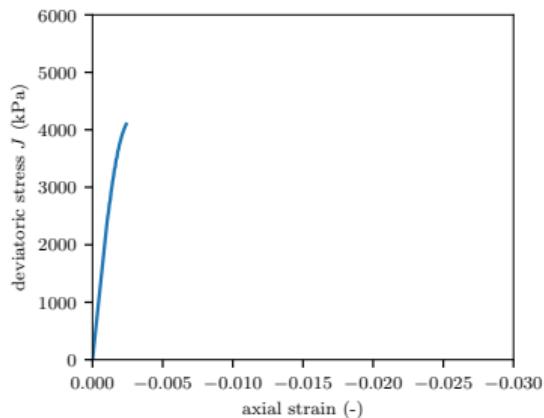
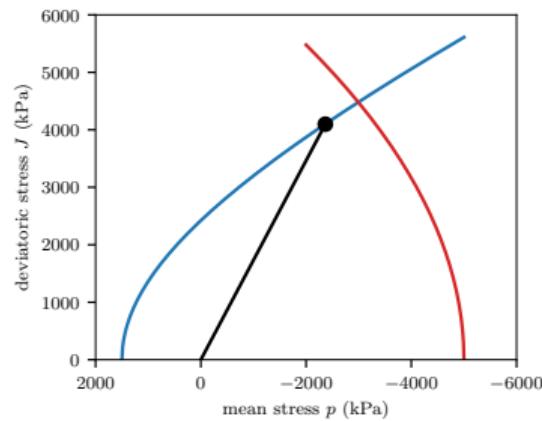
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



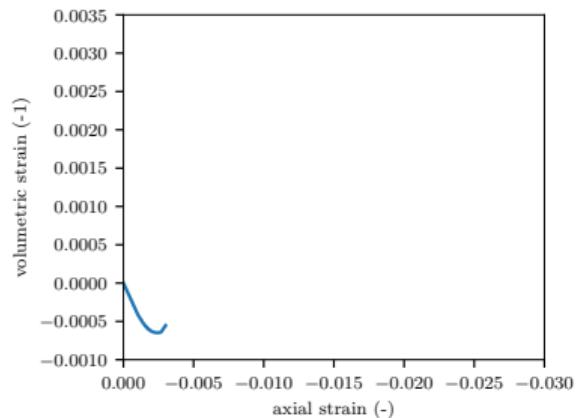
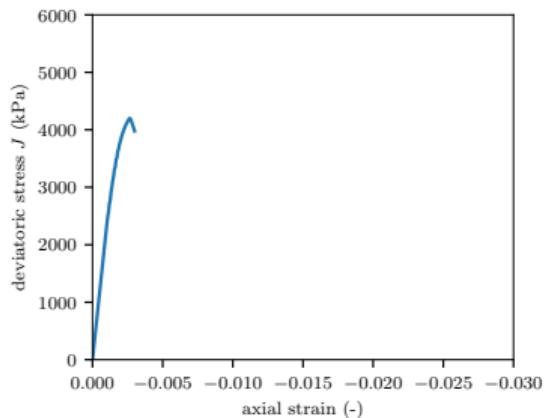
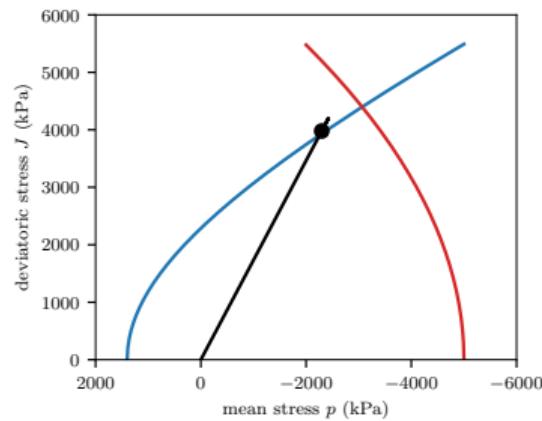
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



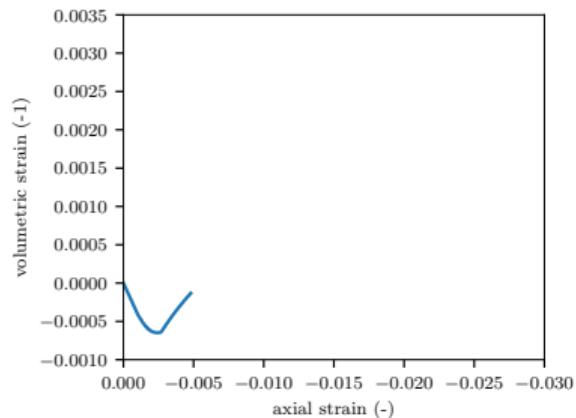
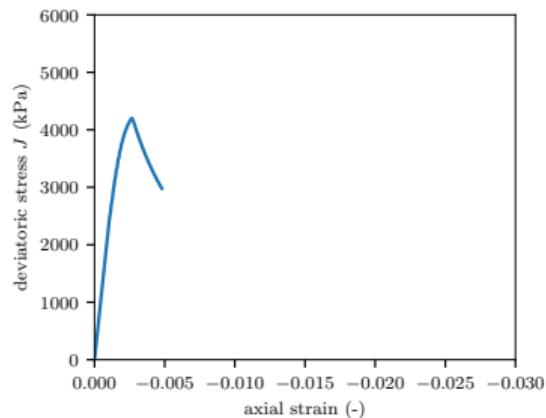
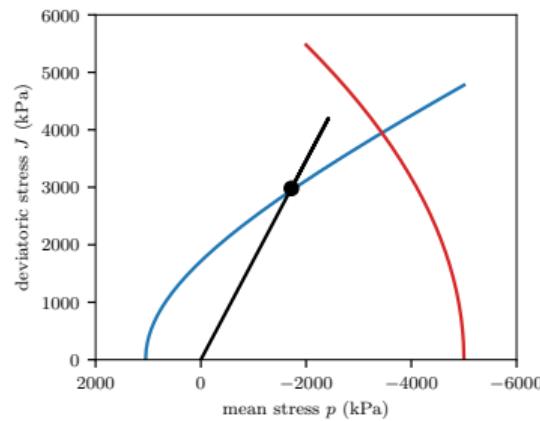
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



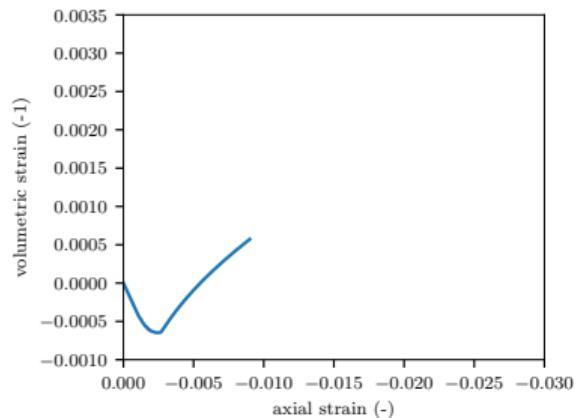
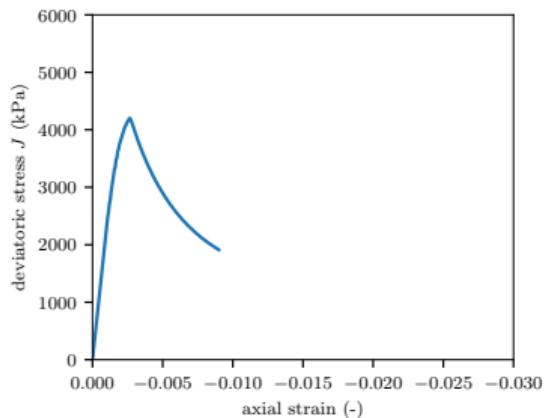
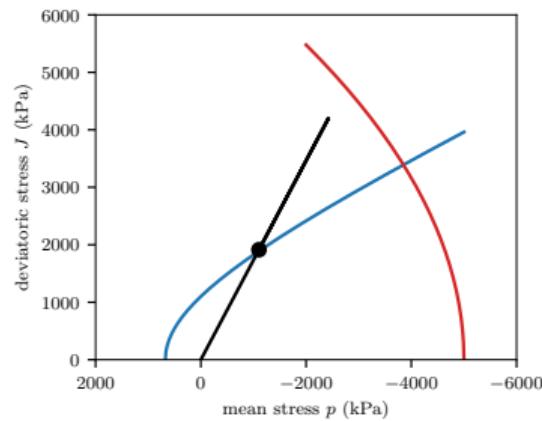
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



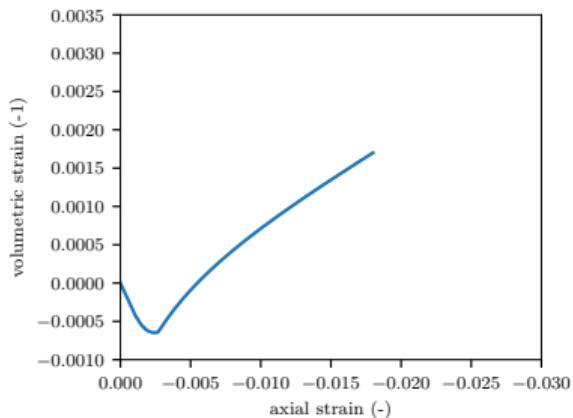
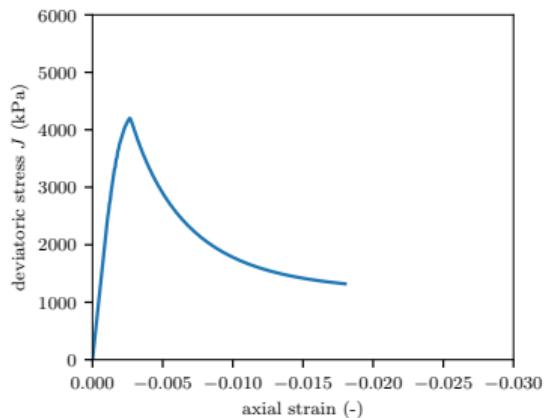
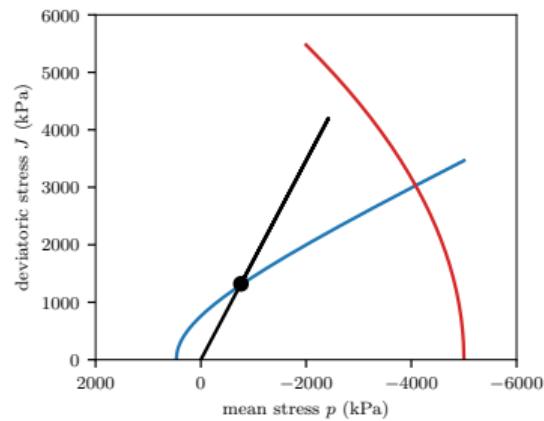
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



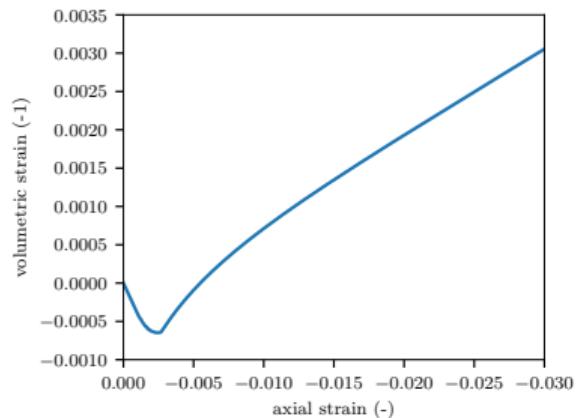
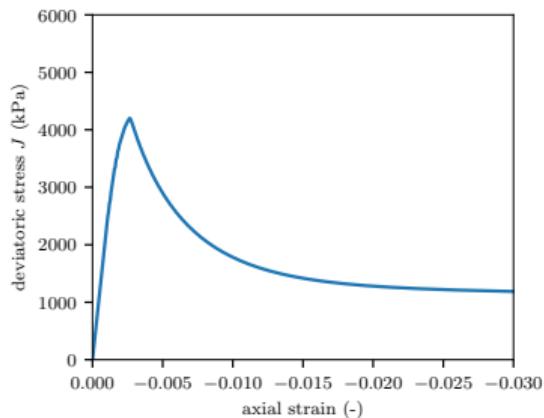
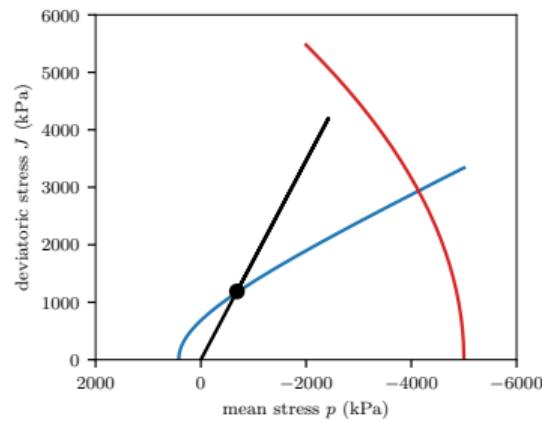
# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*



# Volumetric yield function

*Mobilisation only of the **deviatoric** yield surface*

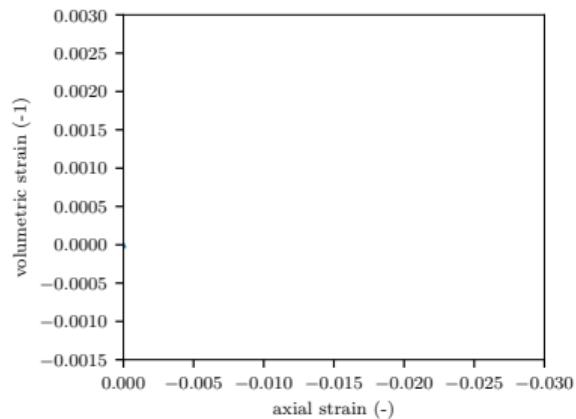
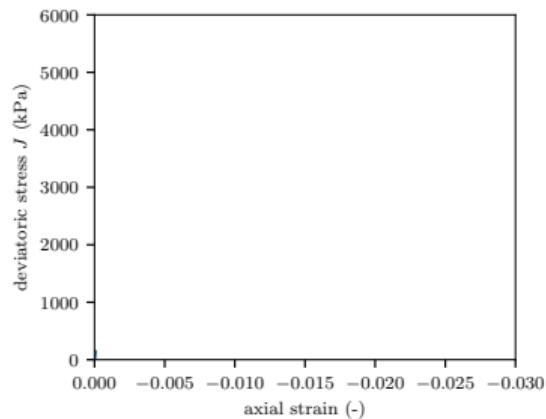
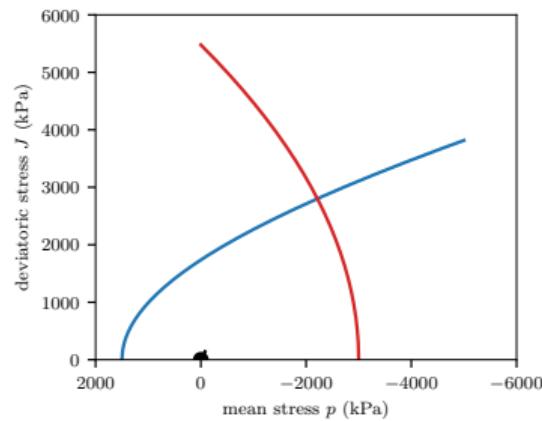


# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*

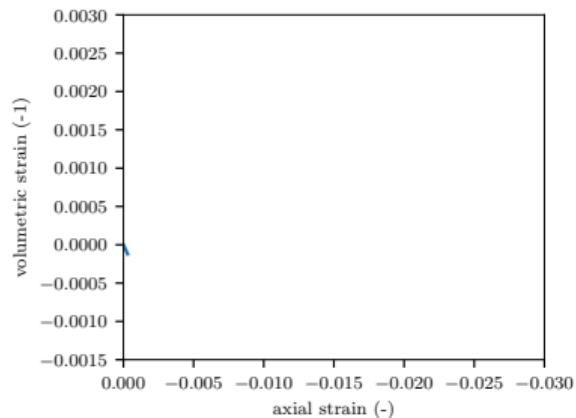
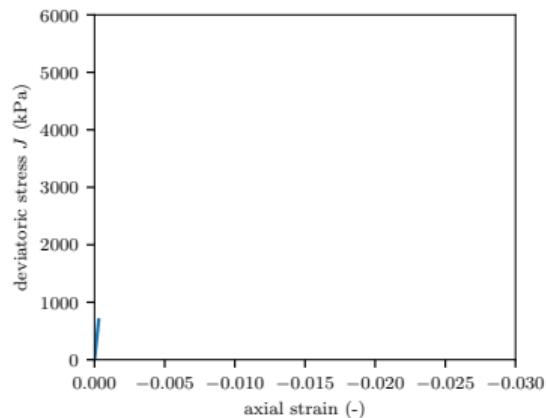
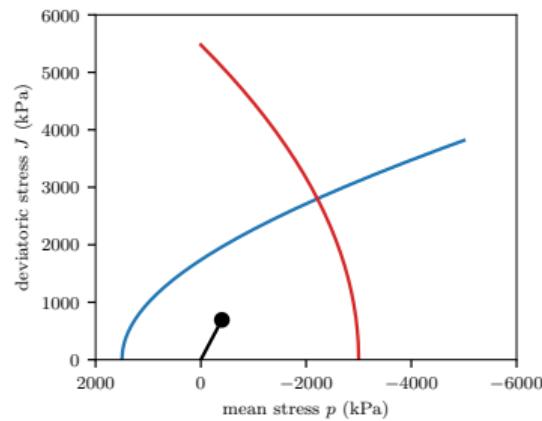
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



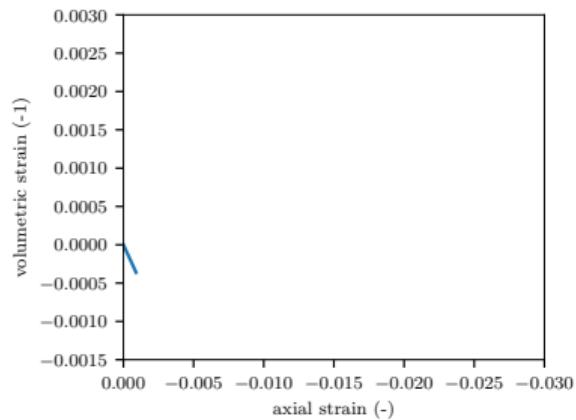
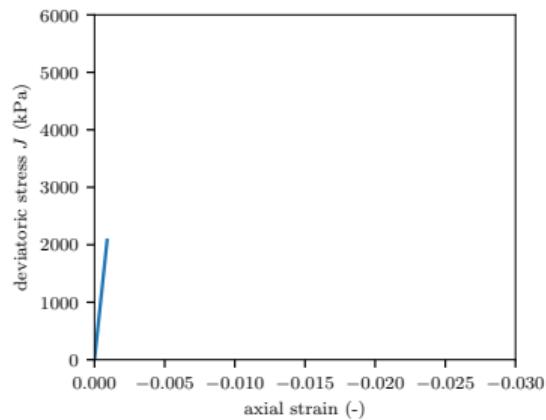
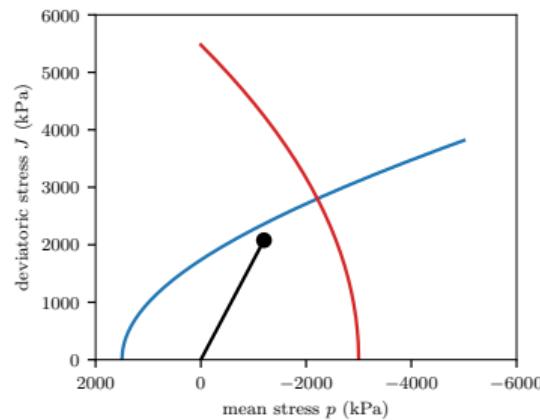
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



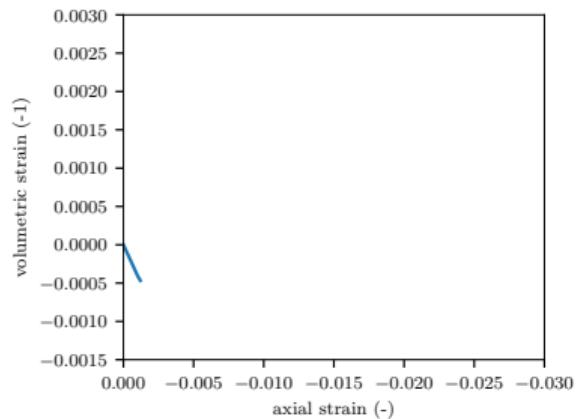
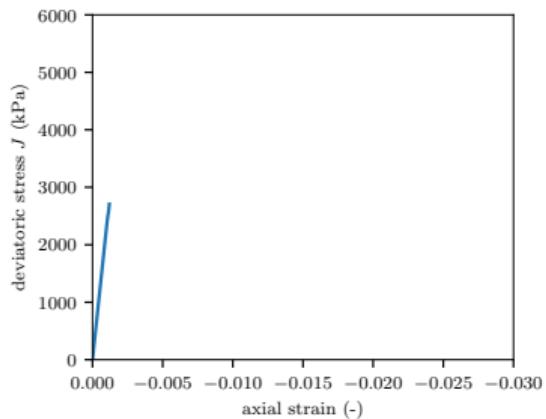
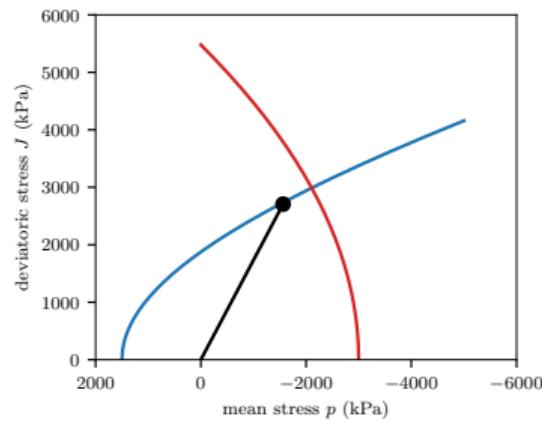
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



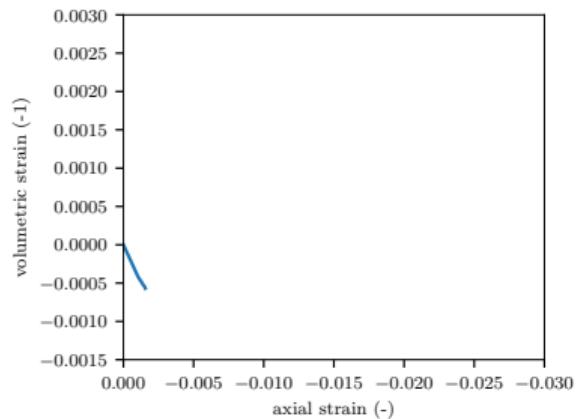
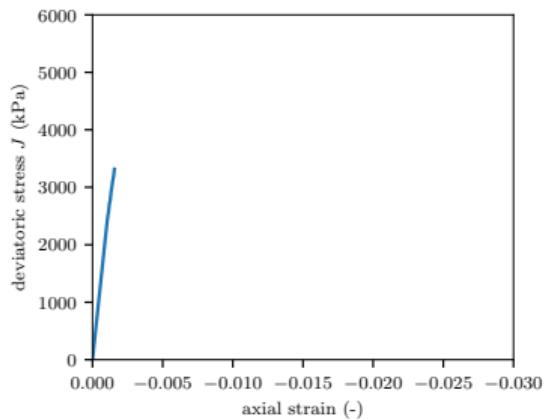
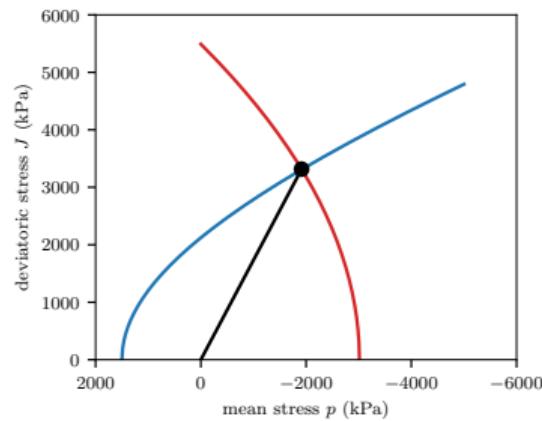
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



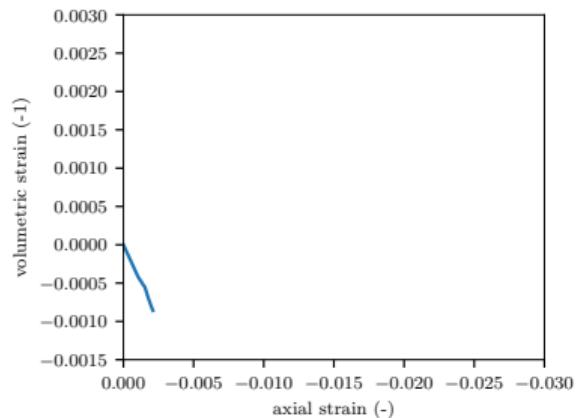
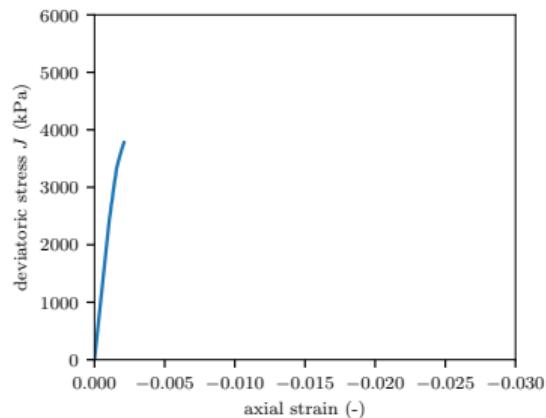
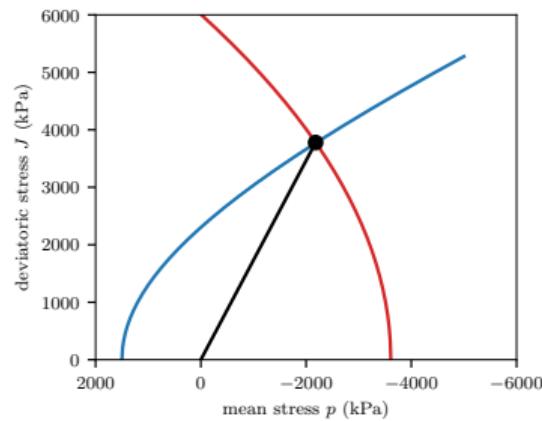
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



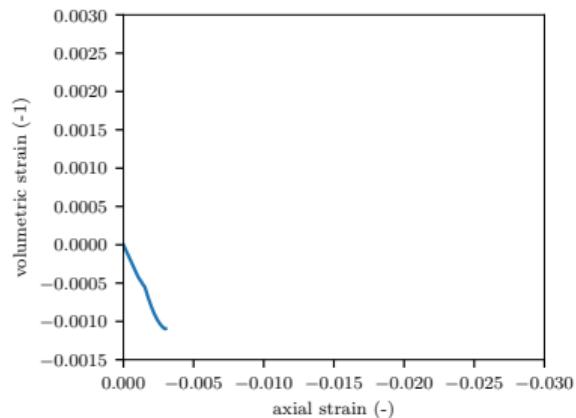
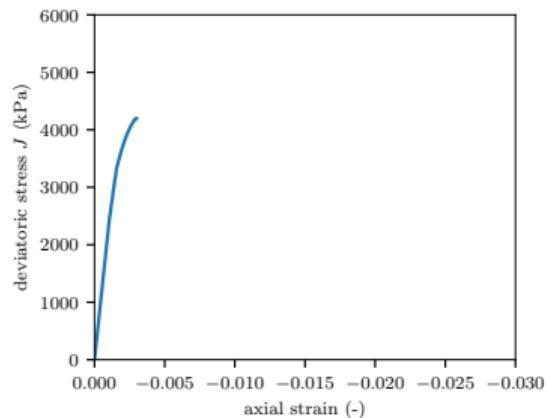
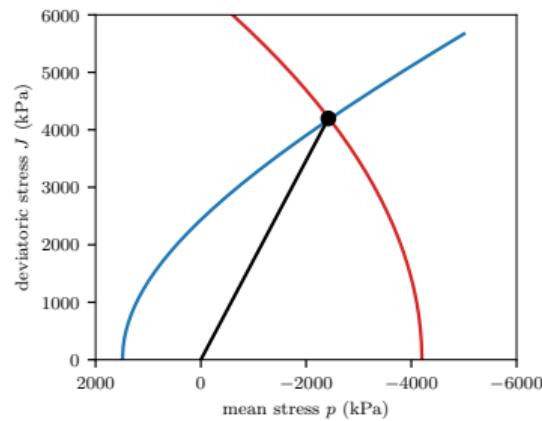
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



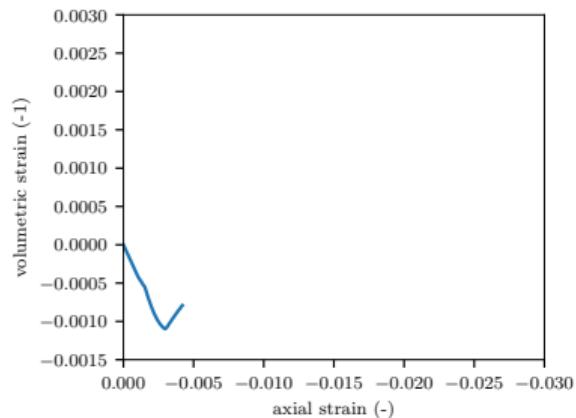
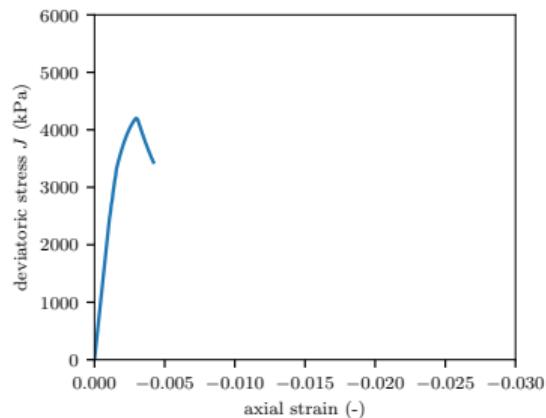
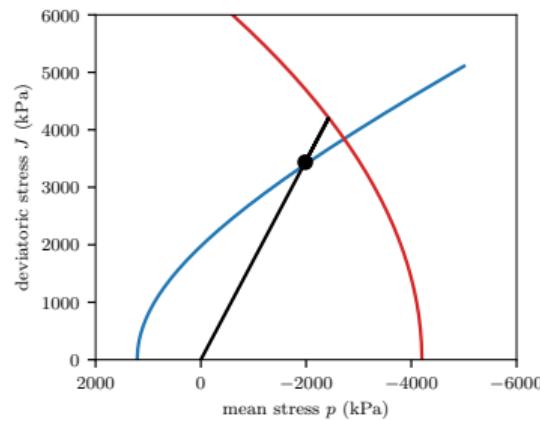
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



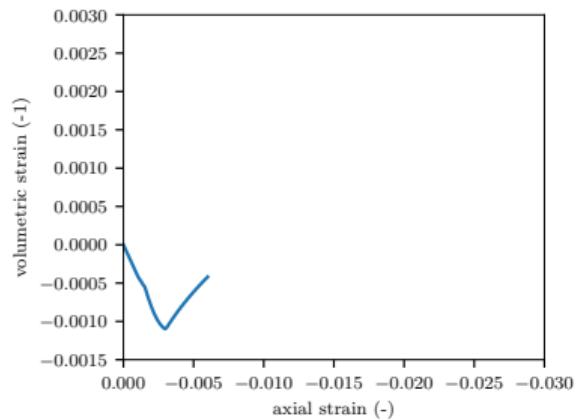
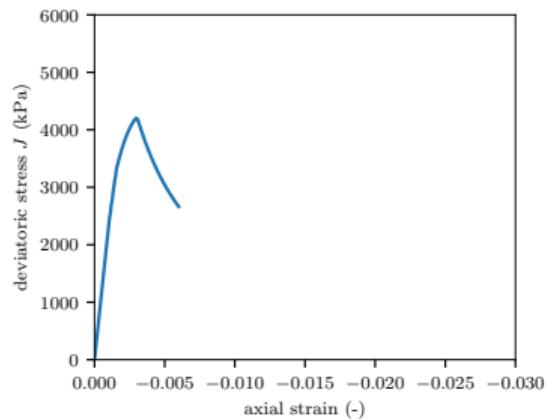
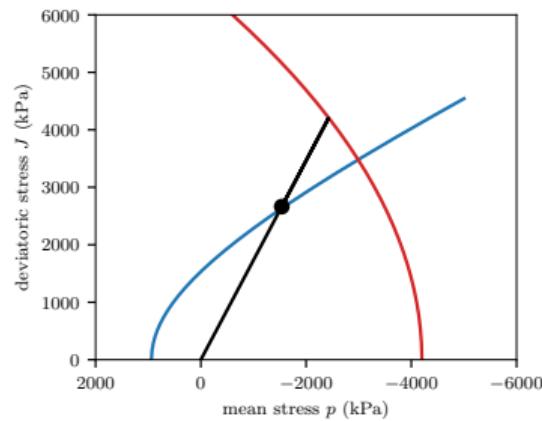
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



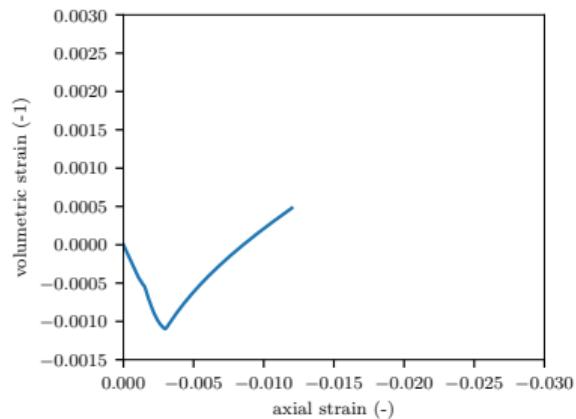
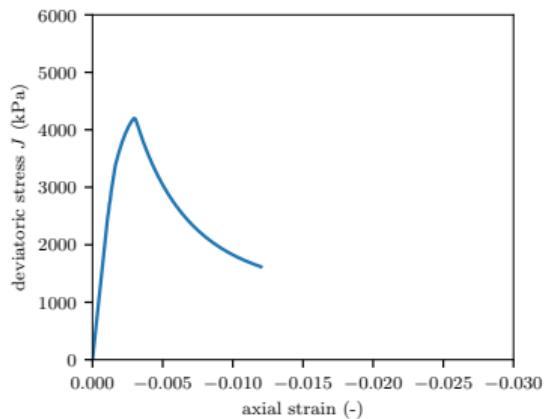
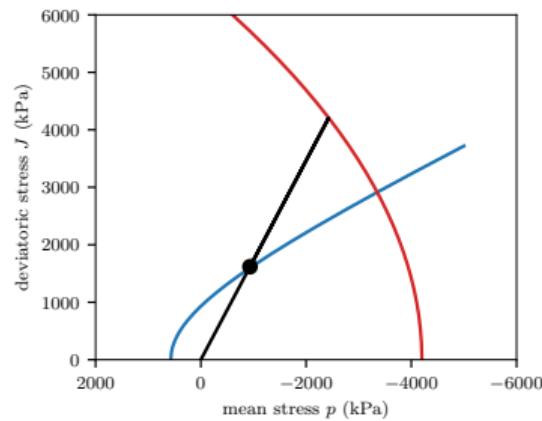
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



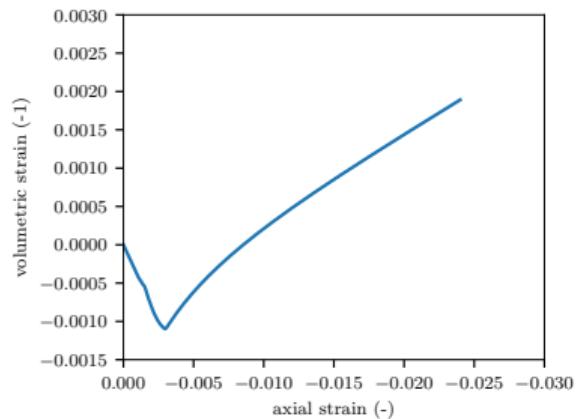
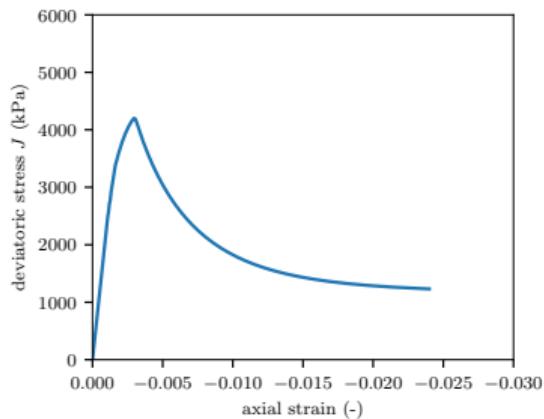
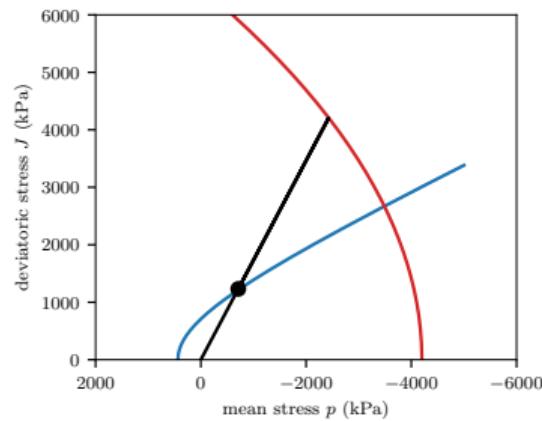
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



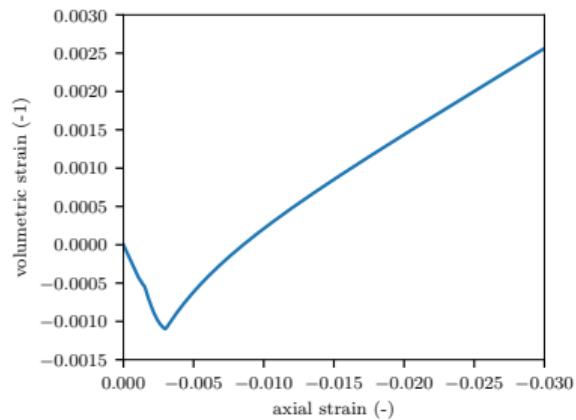
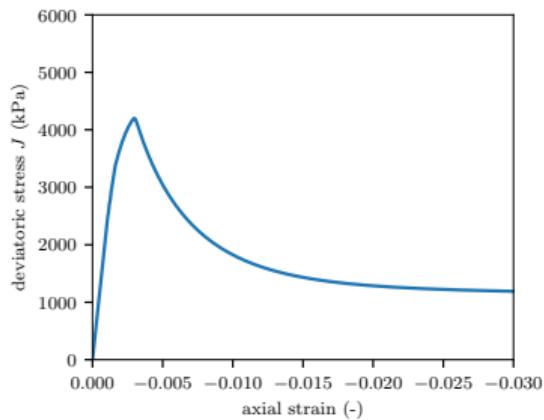
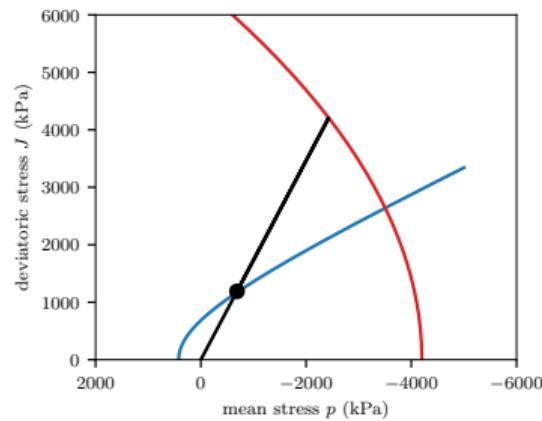
# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*



# Volumetric yield function

*Mobilisation first of the **deviatoric** yield surface and then the **volumetric** yield surface*

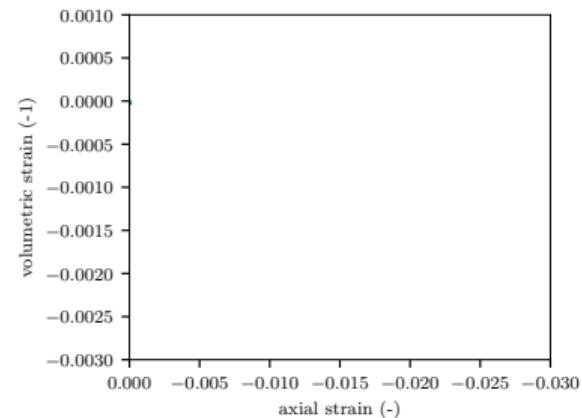
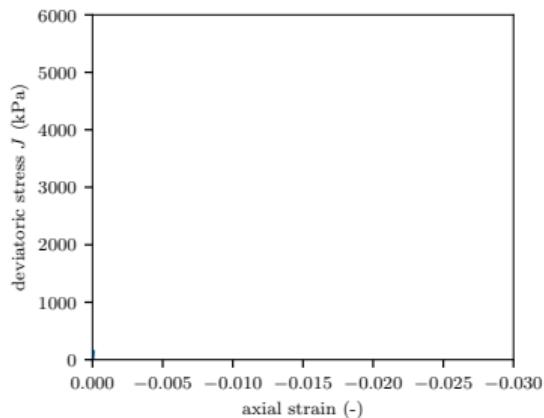
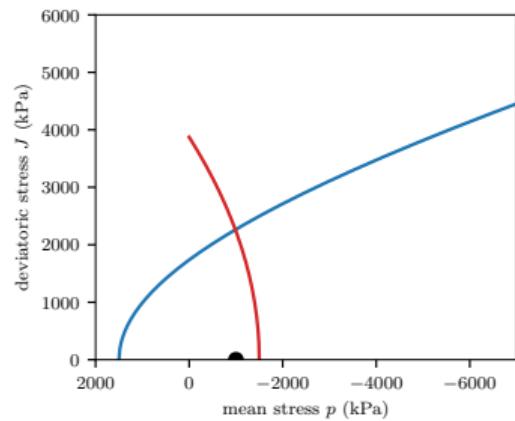


# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*

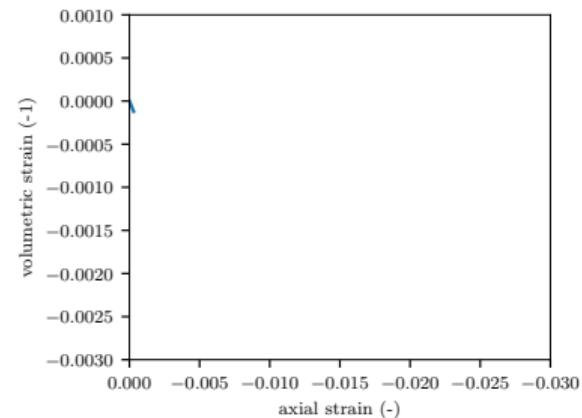
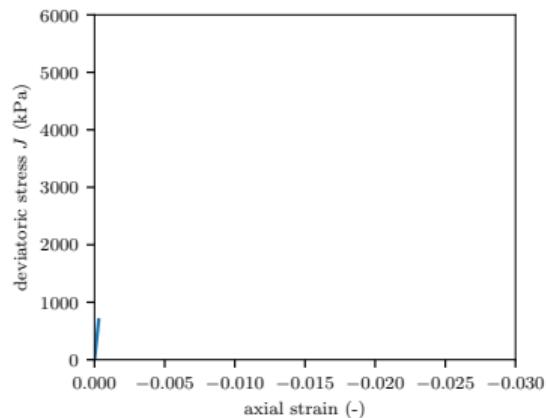
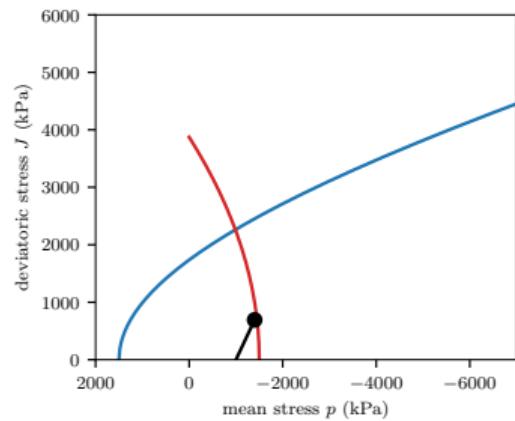
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



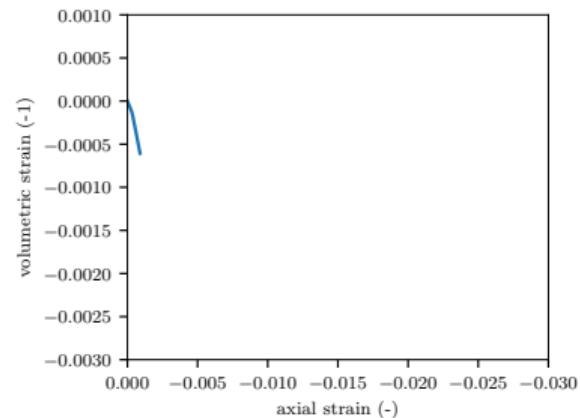
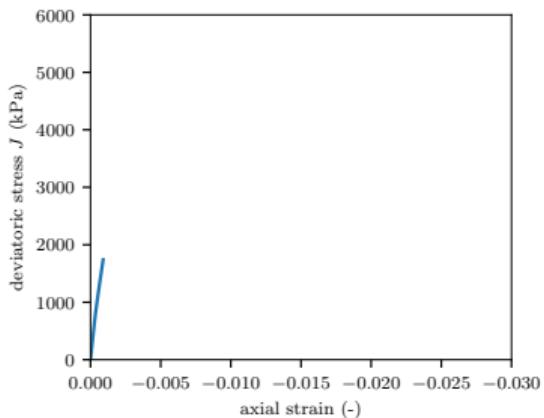
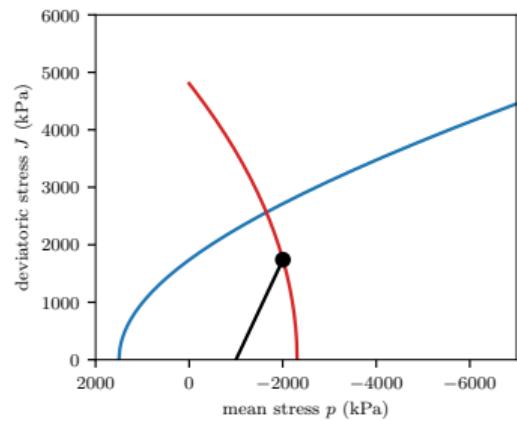
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



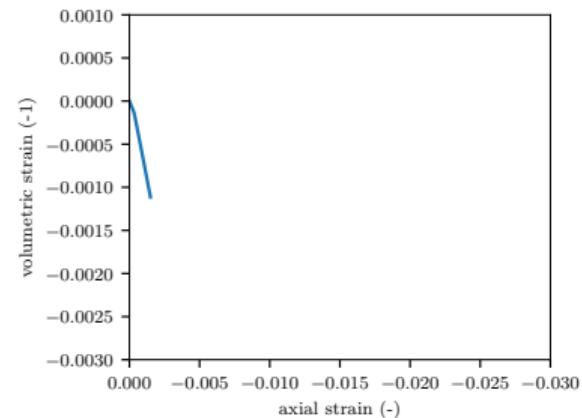
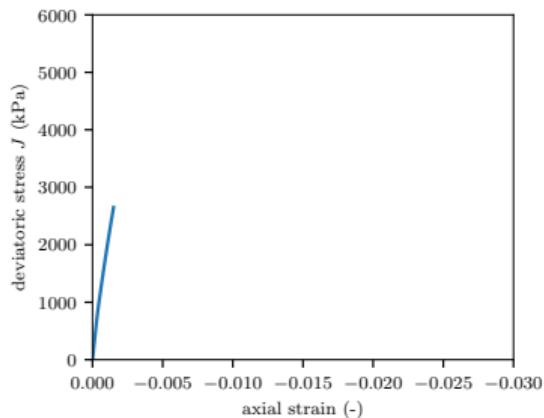
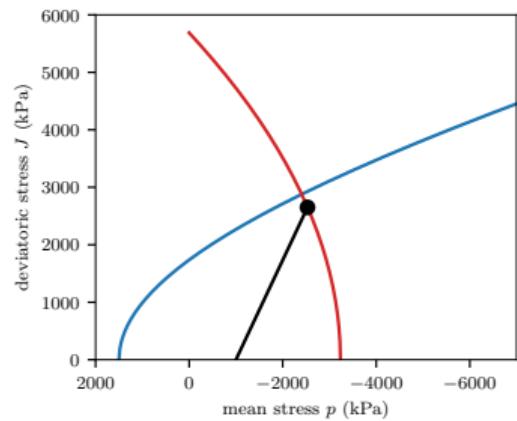
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



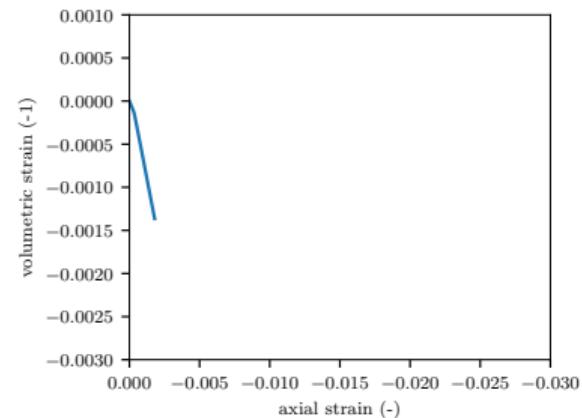
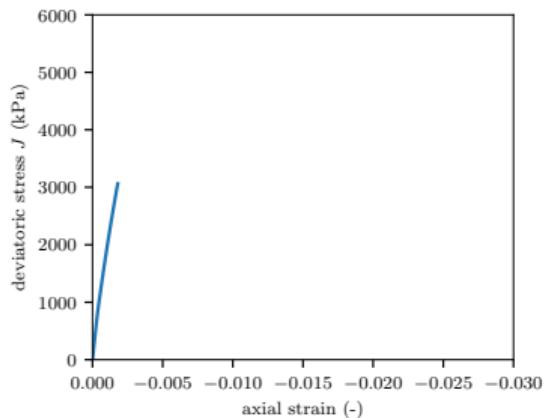
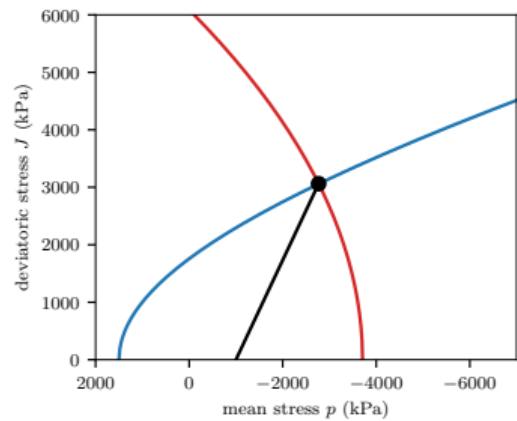
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



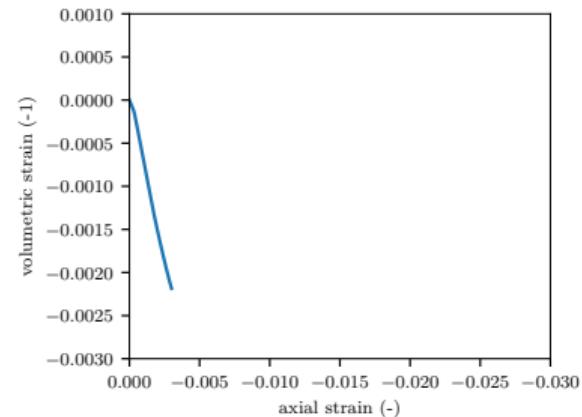
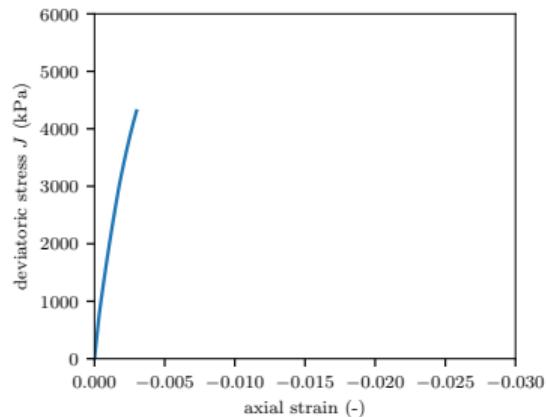
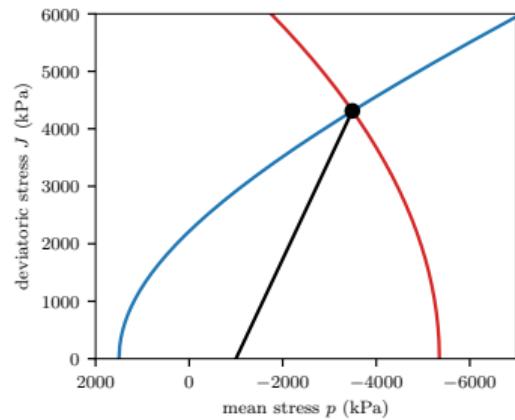
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



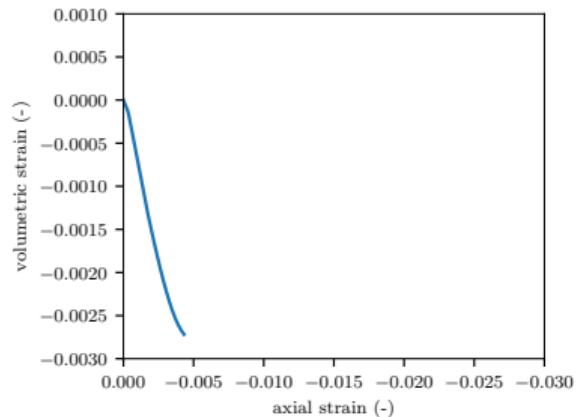
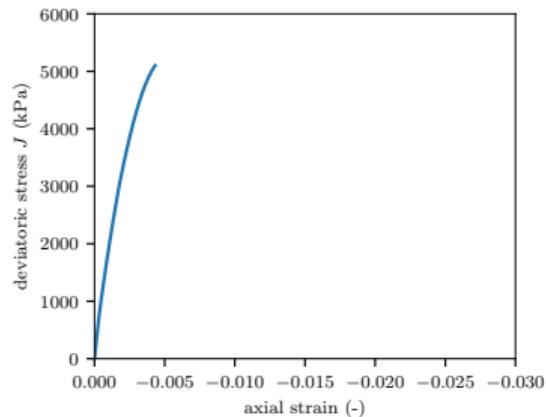
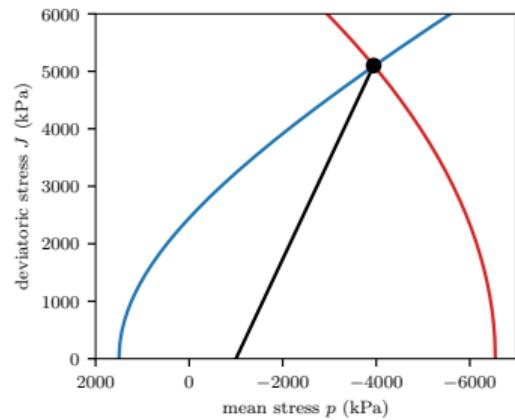
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



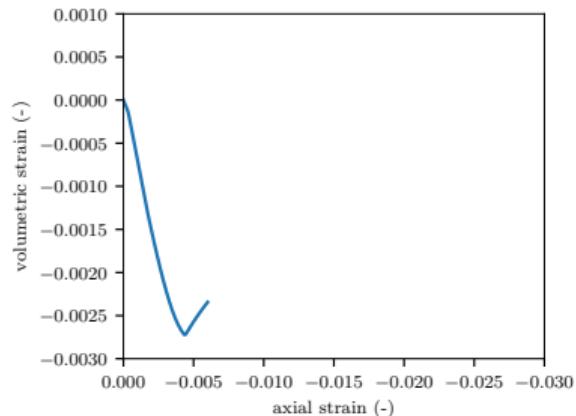
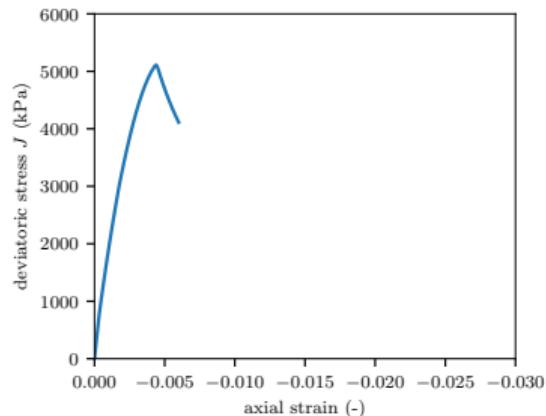
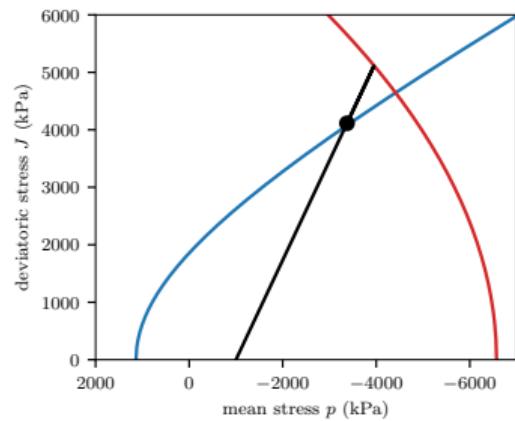
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



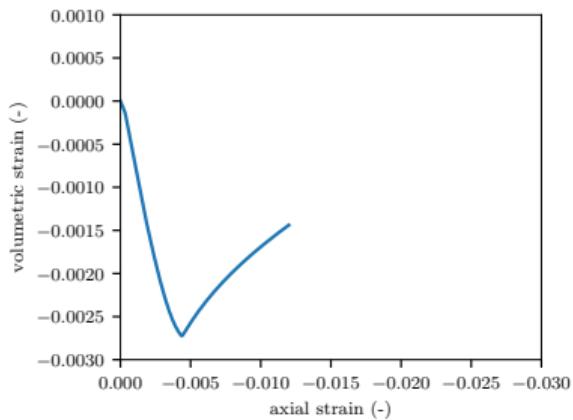
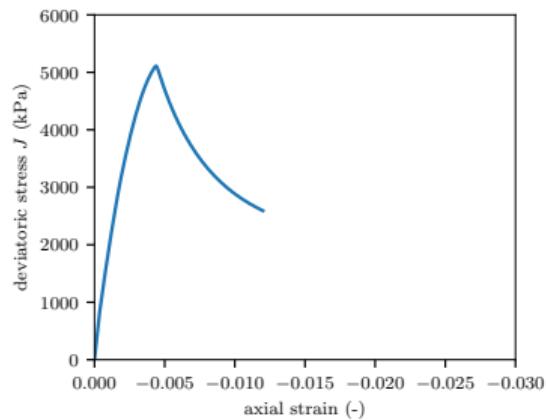
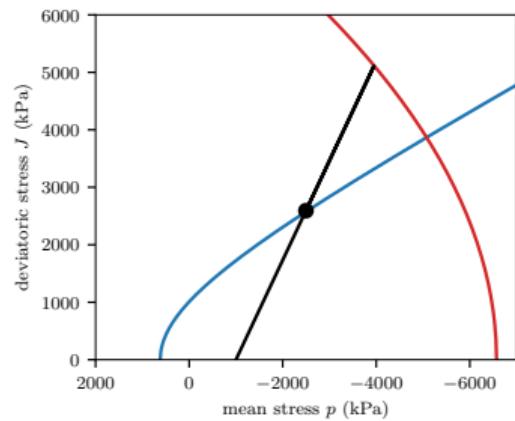
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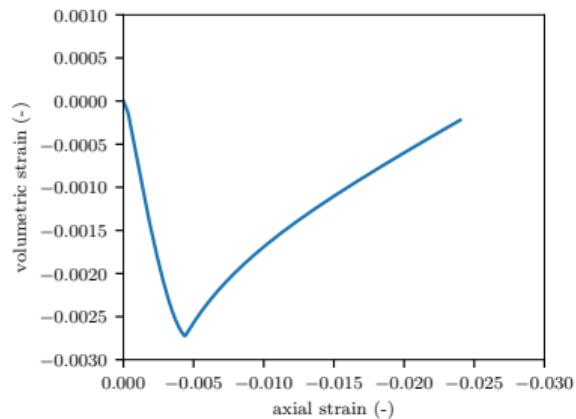
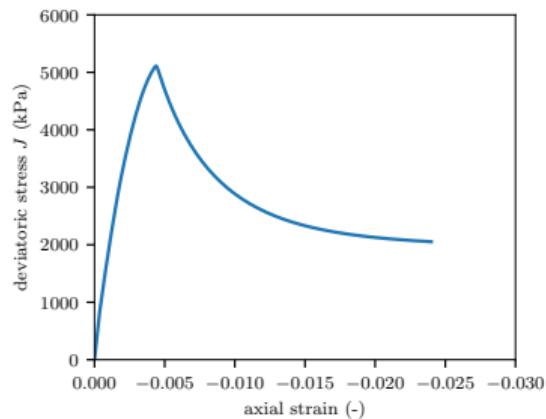
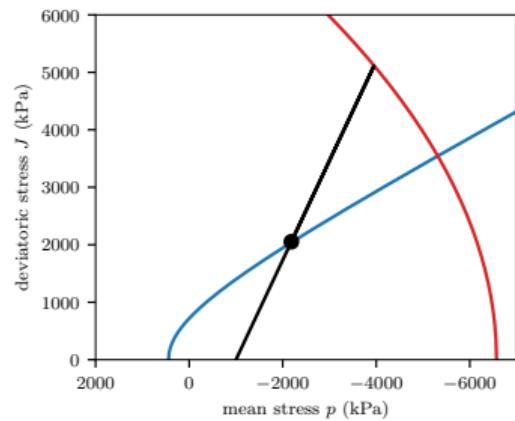
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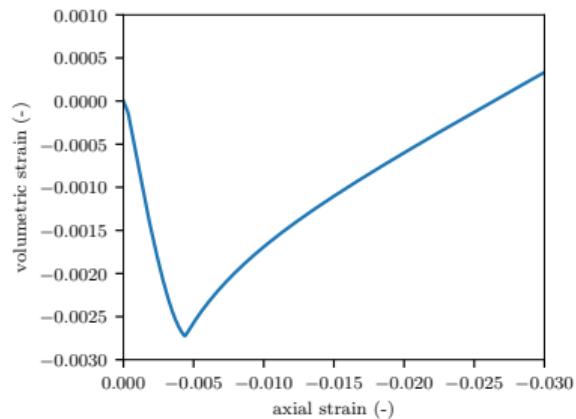
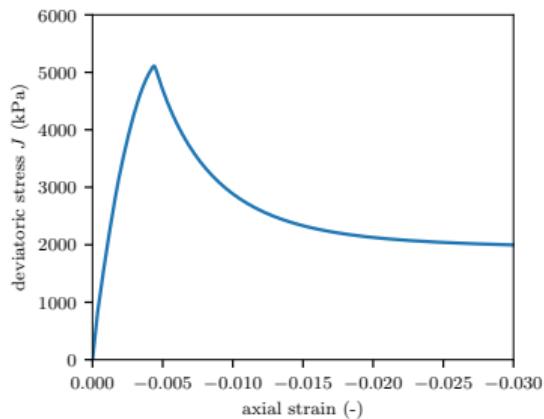
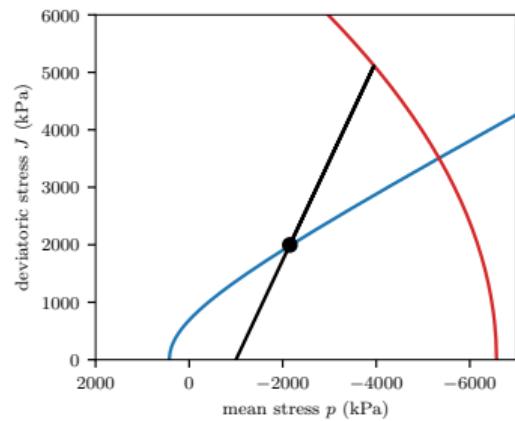
# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



# Volumetric yield function

*Mobilisation first of the **volumetric** yield surface and then the **deviatoric** yield surface*



# Content

## 1 Introduction

## 2 Implementation of thermal effects

- Volumetric yield function
- Temperature dependence of the **deviatoric** yield surface
- Temperature dependence of the **volumetric** yield surface
- Additional convergence checks

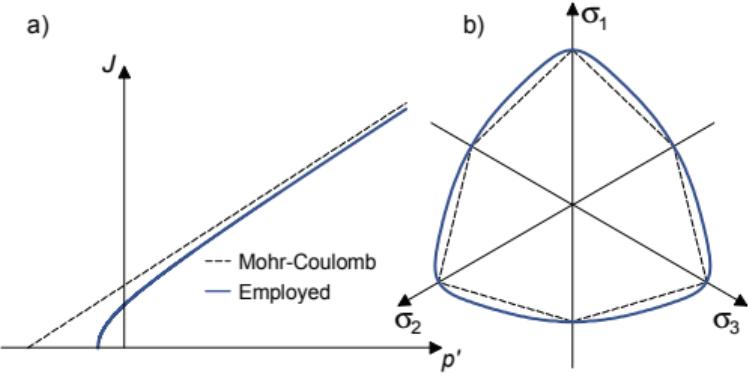
## 3 Coupled THM BVP simulation

## 4 Conclusions

# Temperature dependence of the **deviatoric** yield surface

- Deviatoric yield surface:

$$f = \sqrt{\frac{J_2}{f_d(\theta)} + (c^* + p_t \tan \phi^*)^2} - (c^* + p' \tan \phi^*)$$



## Temperature dependence of the **deviatoric** yield surface

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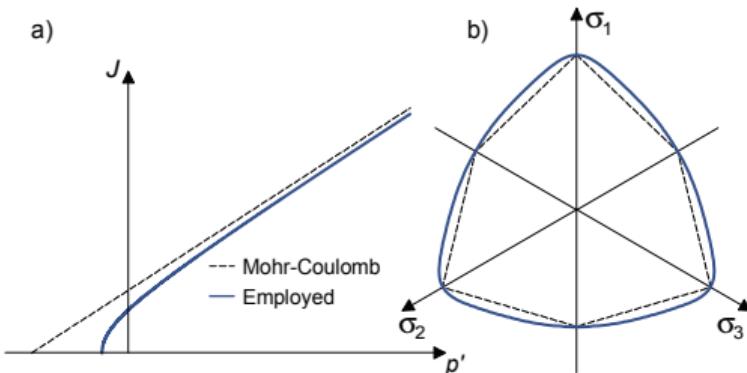
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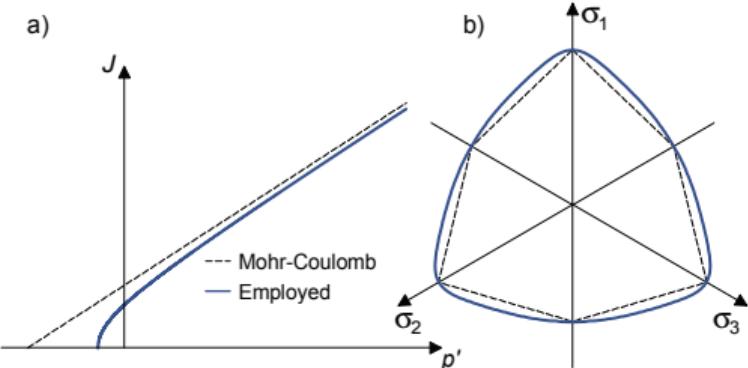
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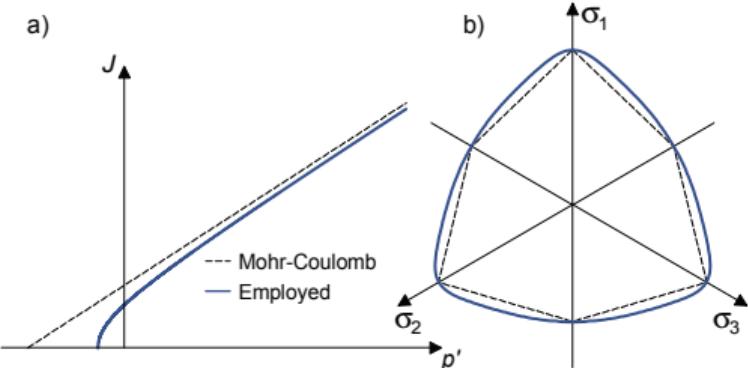
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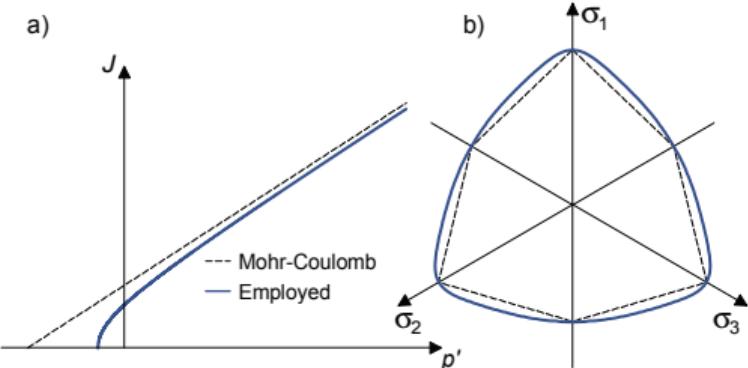
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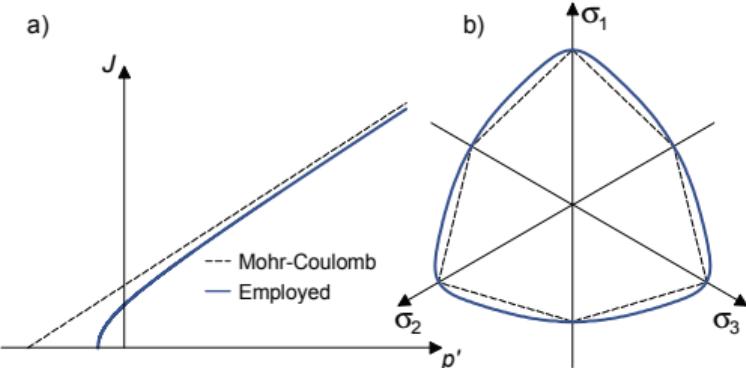
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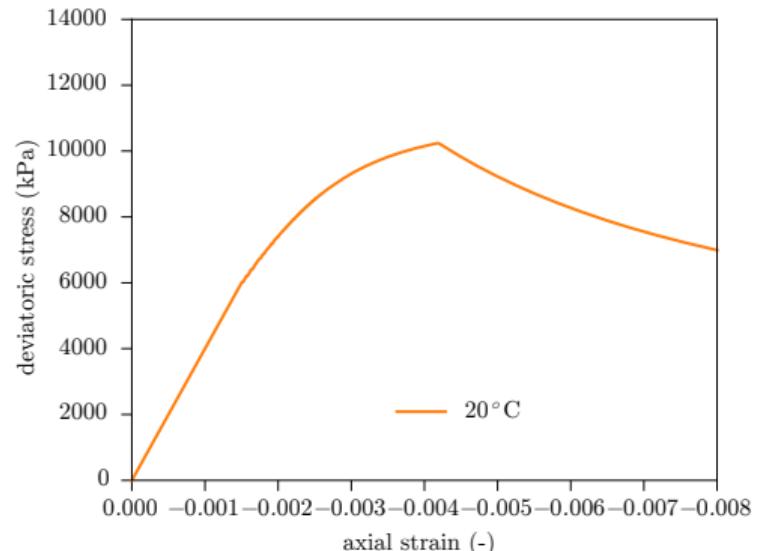
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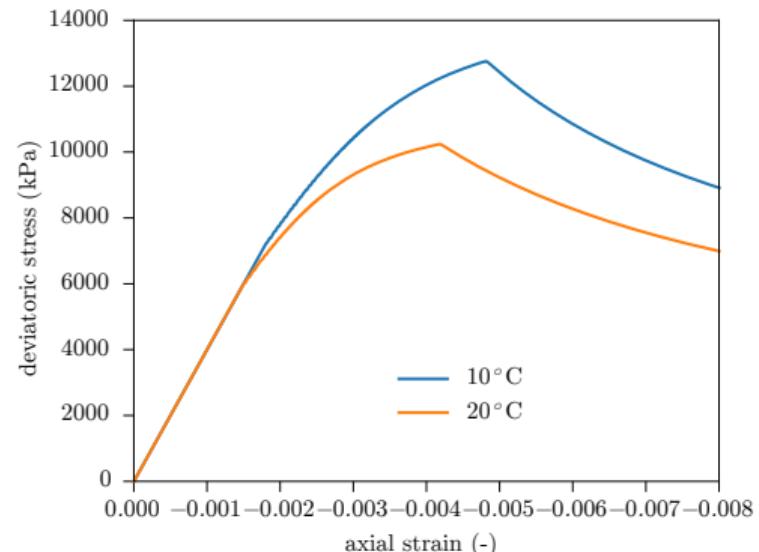
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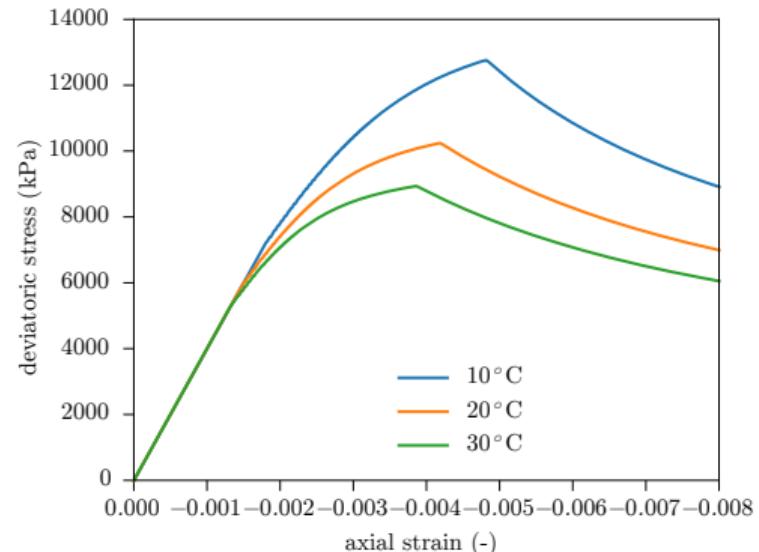
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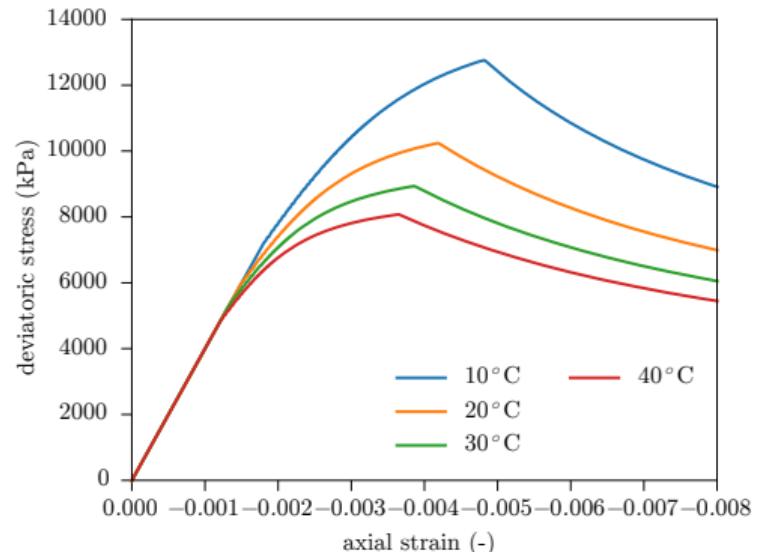
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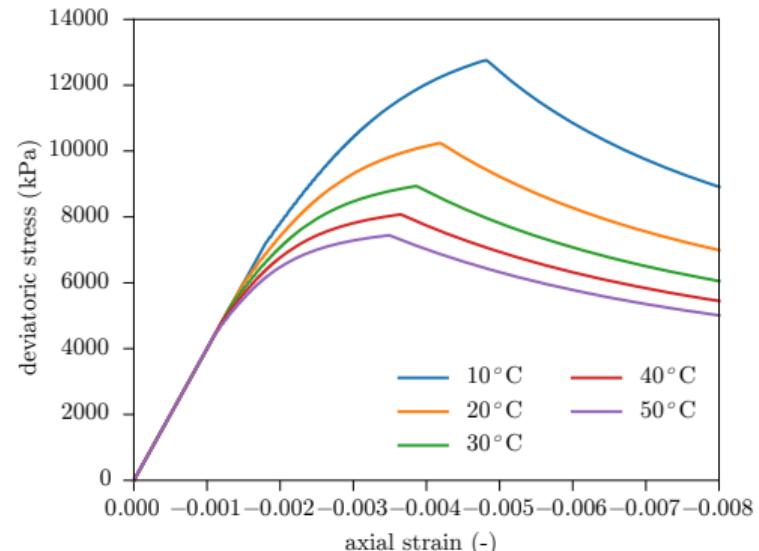
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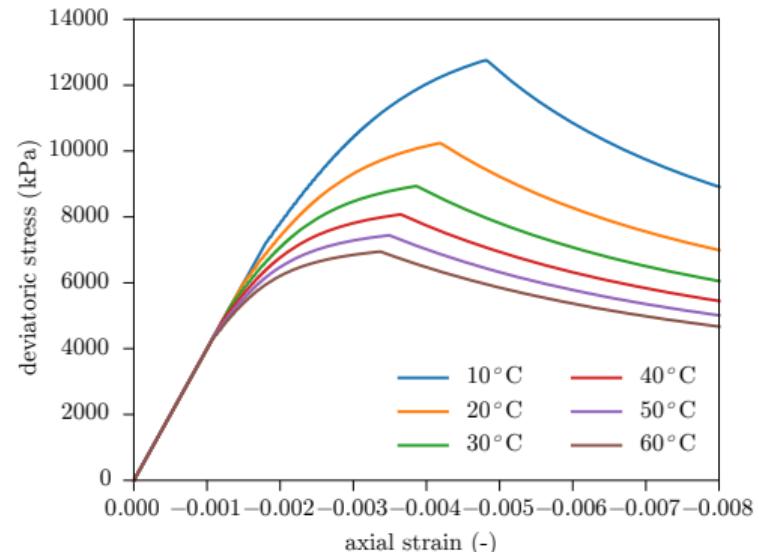
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# Content

## 1 Introduction

## 2 Implementation of thermal effects

- Volumetric yield function
- Temperature dependence of the **deviatoric** yield surface
- **Temperature dependence of the **volumetric** yield surface**
- Additional convergence checks

## 3 Coupled THM BVP simulation

## 4 Conclusions

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- Volumetric yield surface:

$$f_2 = \frac{J^2}{R} + p_c - p_{c0} T_0 [1 - \mu_{p_c} \ln(T/T_0)] - p$$

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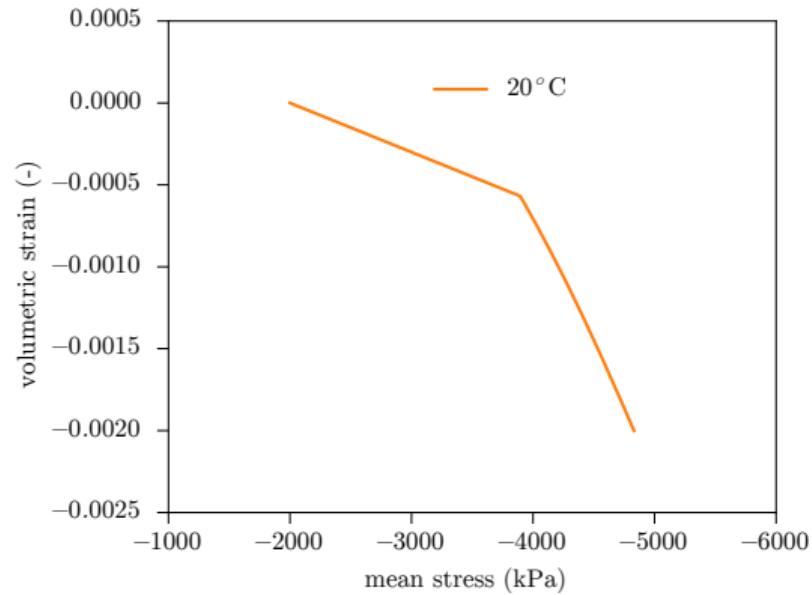
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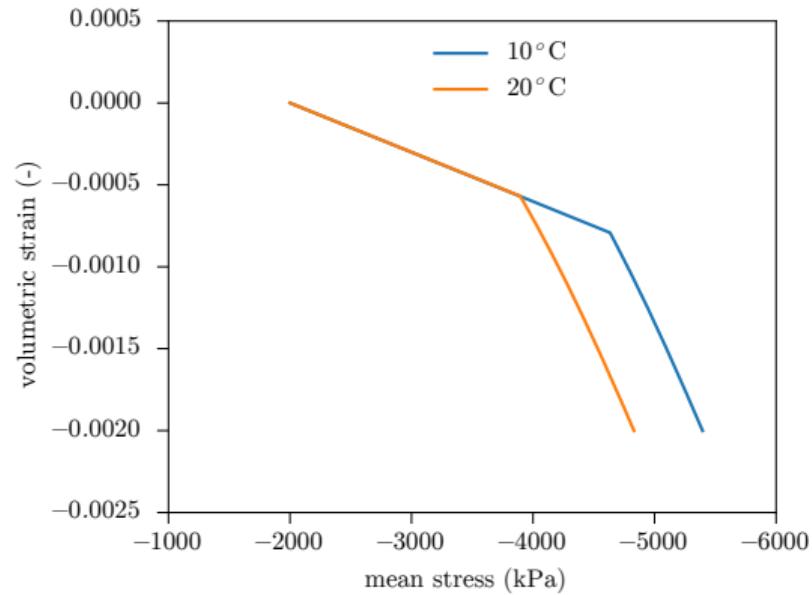
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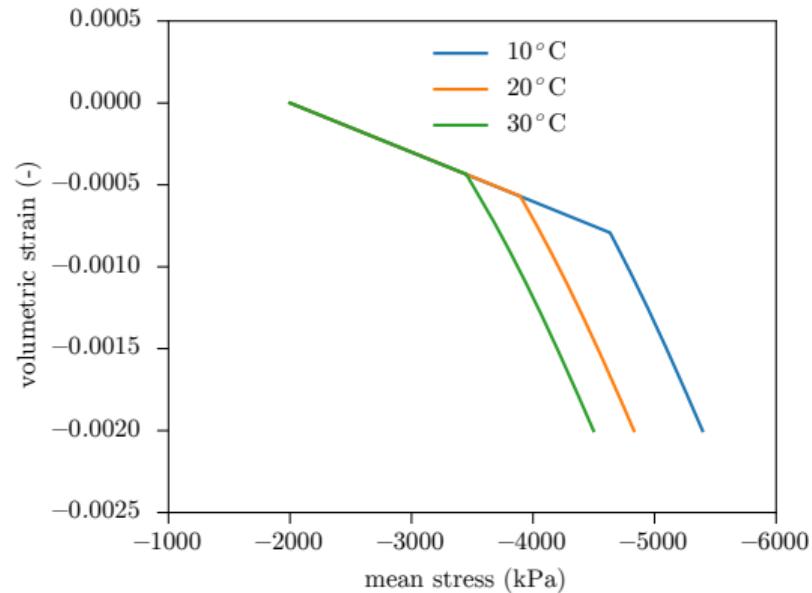
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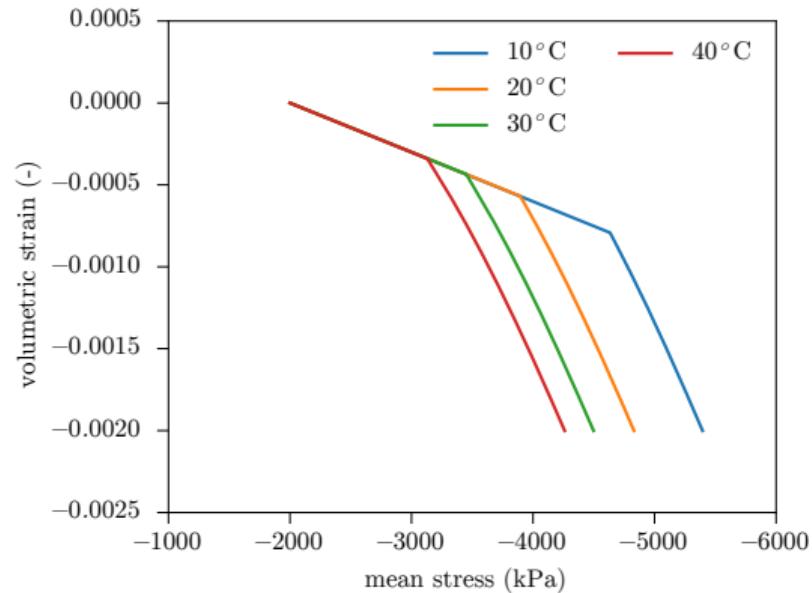
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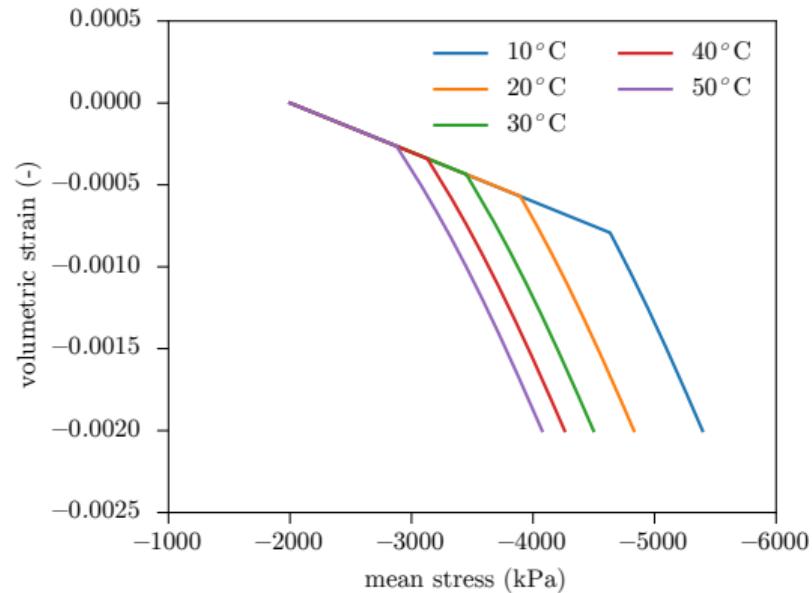
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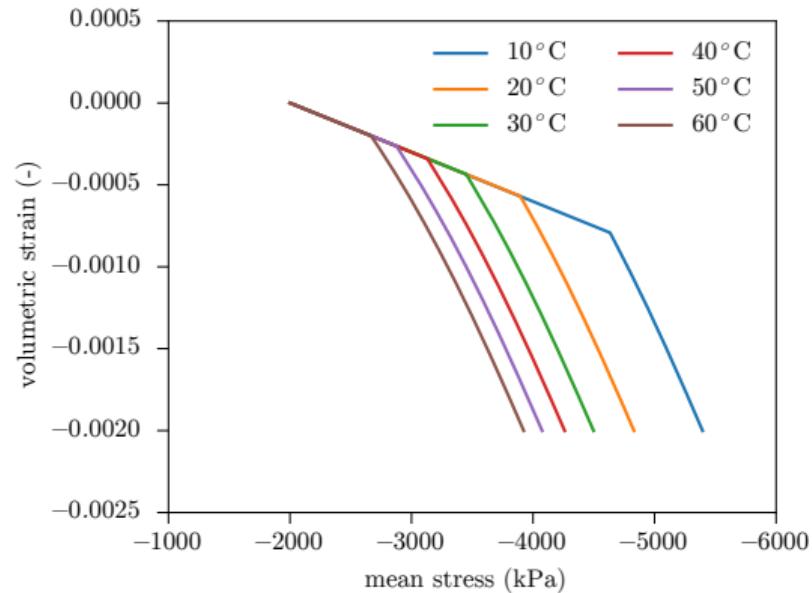
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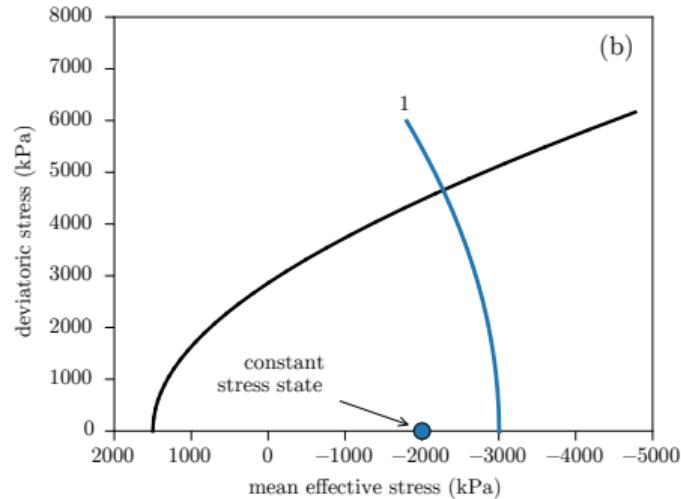
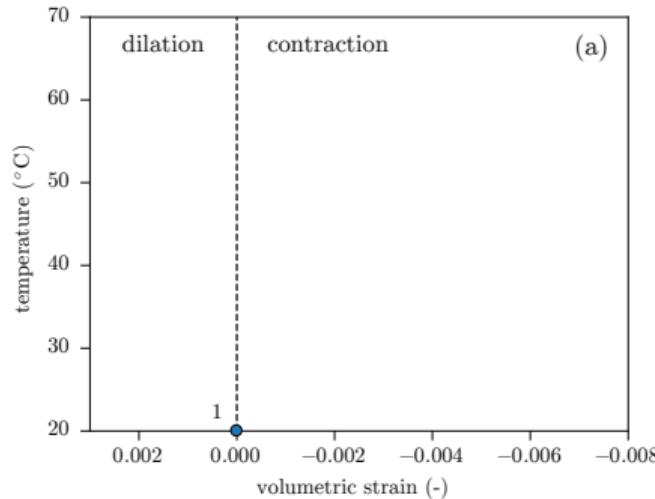
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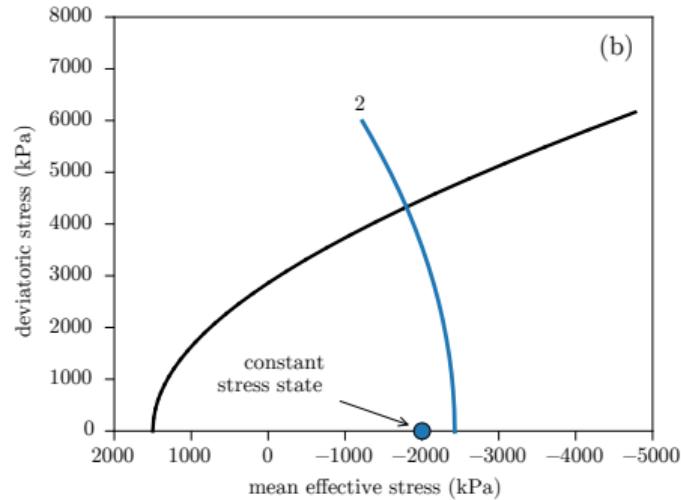
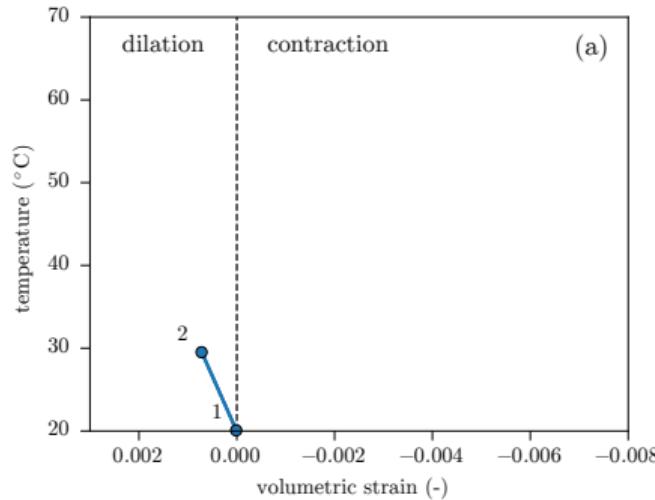
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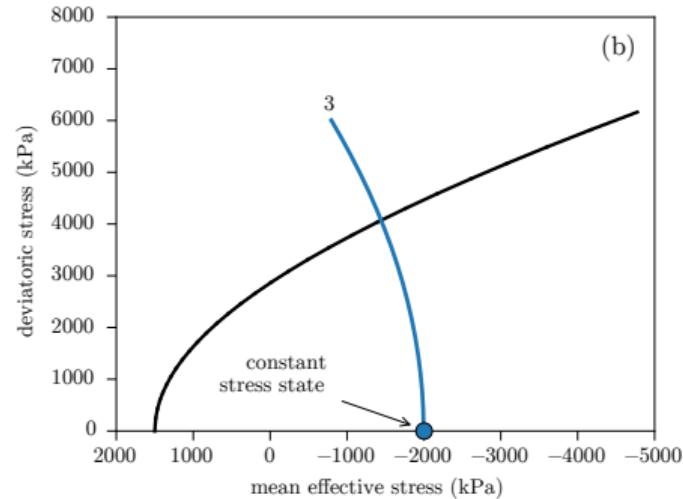
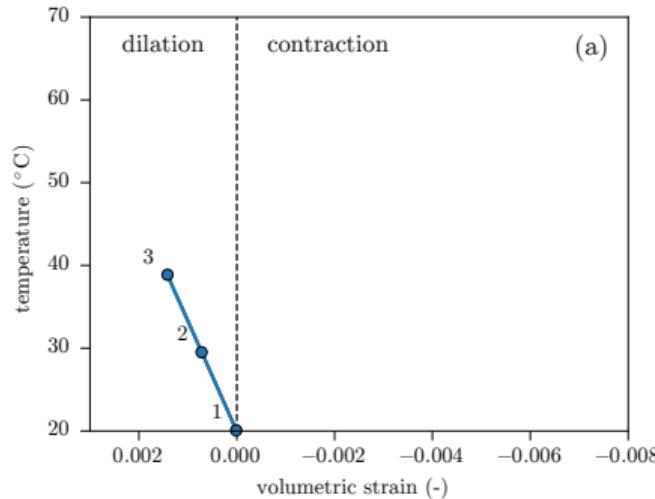
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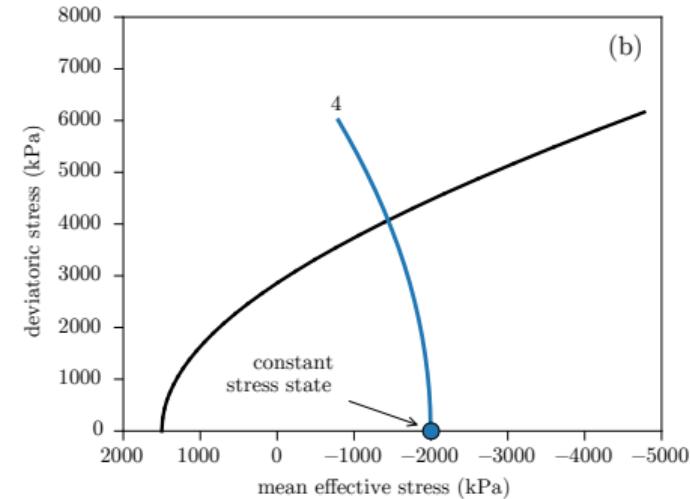
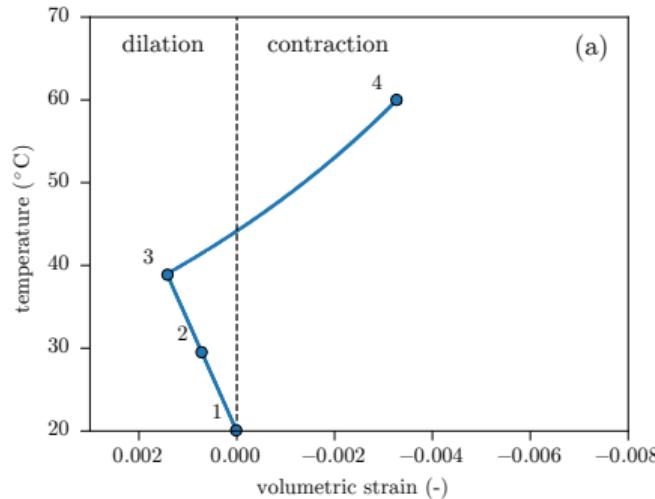
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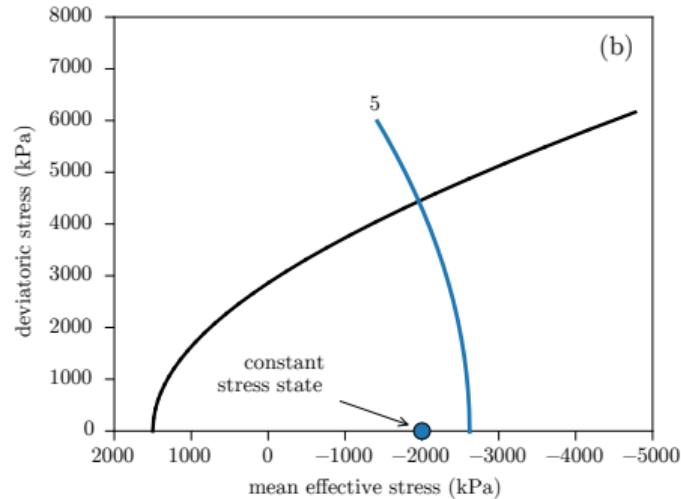
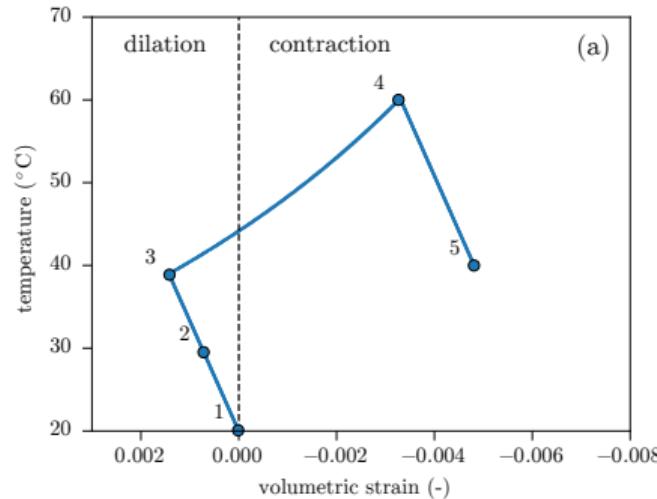
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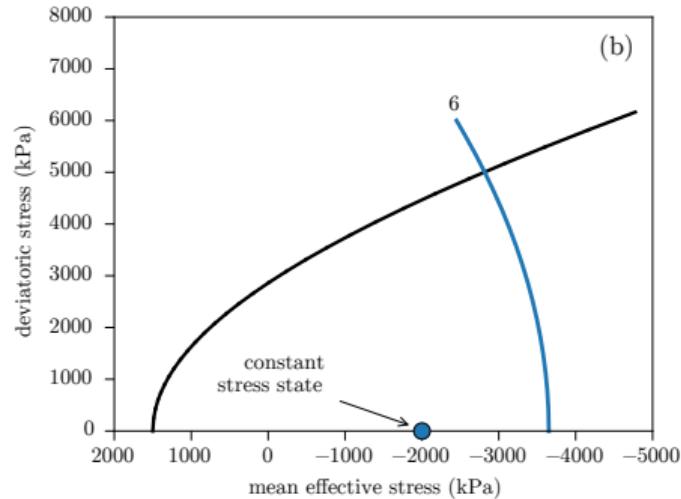
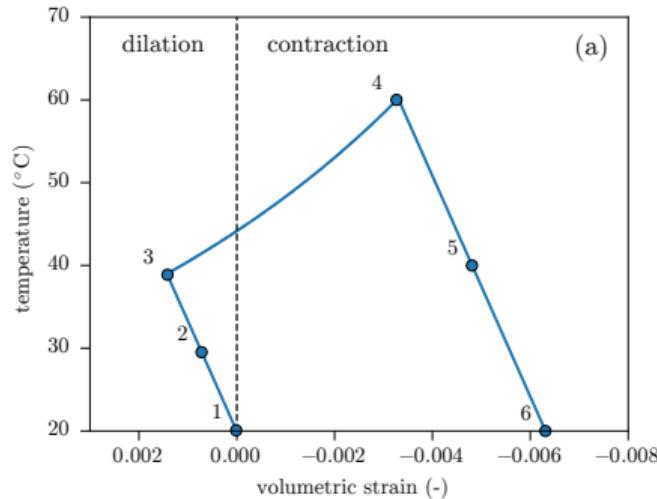
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# Content

## 1 Introduction

## 2 Implementation of thermal effects

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## 3 Coupled THM BVP simulation

## 4 Conclusions

# Additional convergence checks

```
@AdditionalConvergenceChecks{
    // check integration type
    bool int_check = false;
    if((f > 0.0) && (f2 < 0.0) && (int_type_1 == false)){int_check = true;}
    if((f < 0.0) && (f2 > 0.0) && (int_type_2 == false)){int_check = true;}
    if((f > 0.0) && (f2 > 0.0) && (int_type_3 == false)){int_check = true;}
    if((f < 0.0) && (f2 < 0.0) && (int_type_4 == false) && (eps_eq_p > eps_thr)){
        int_check = true;
    }
    if(int_check){
        converged = false;
        int_type_1 = false;
        int_type_2 = false;
        int_type_3 = false;
        int_type_4 = false;
        if((f > 0.0) && (f2 < 0.0)){int_type_1 = true;}
        if((f < 0.0) && (f2 > 0.0)){int_type_2 = true;}
        if((f > 0.0) && (f2 > 0.0)){int_type_3 = true;}
        if((f < 0.0) && (f2 < 0.0) && (eps_eq_p > eps_thr)){int_type_4 = true;}
    }
}
```

# Content

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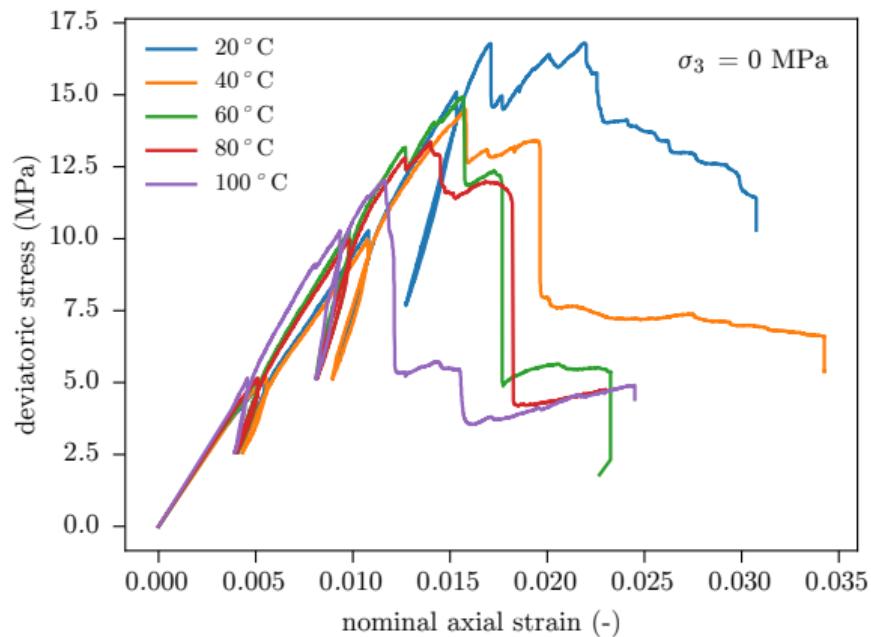
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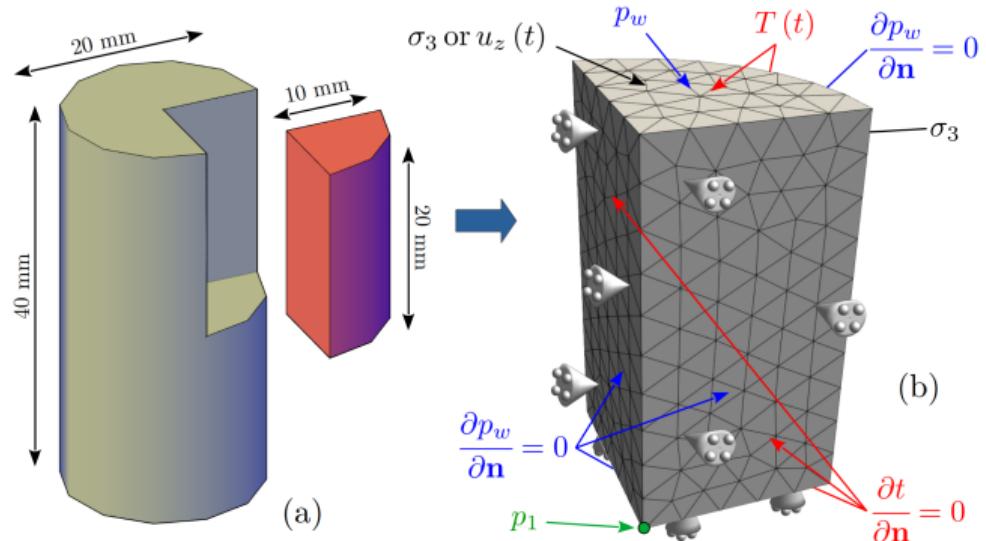
# Coupled THM BVP simulation

- Simulation of triaxial tests with temperature control in the context of the HITEC project.



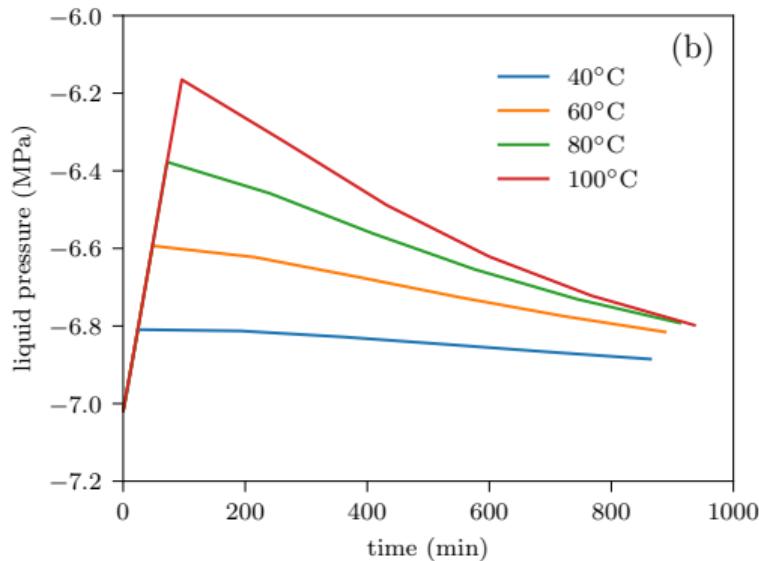
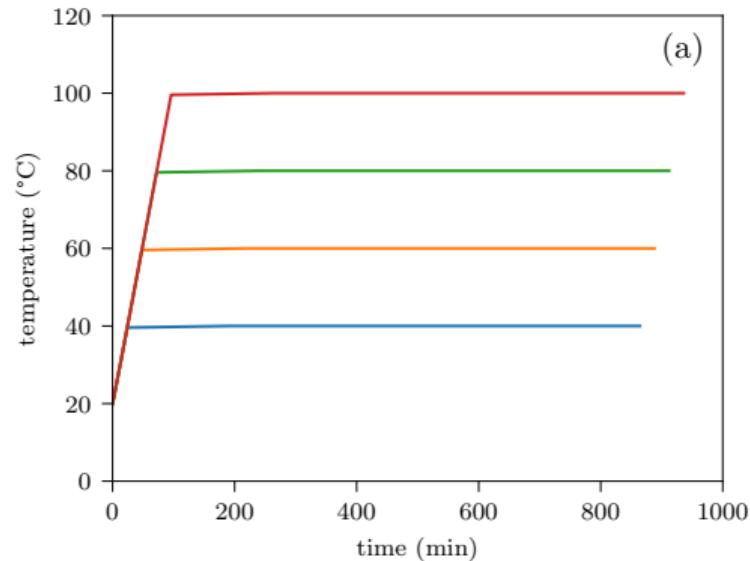
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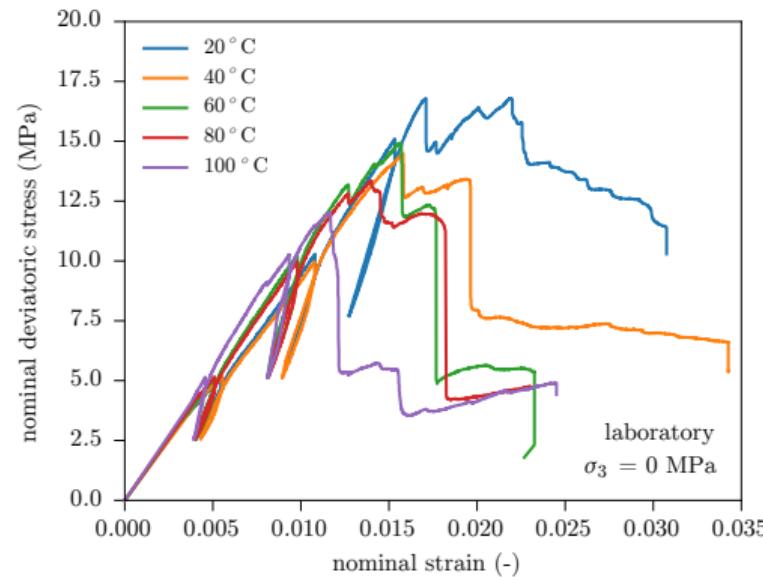
# Coupled THM BVP simulation

*Obtained results*



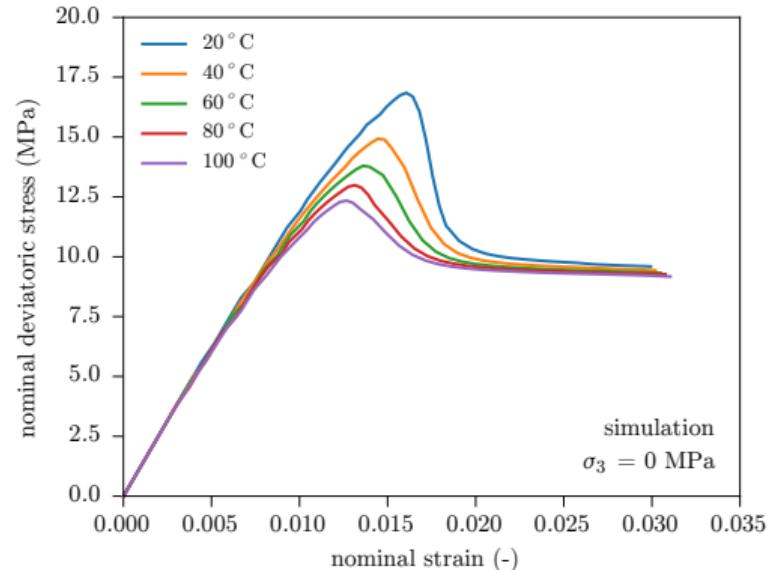
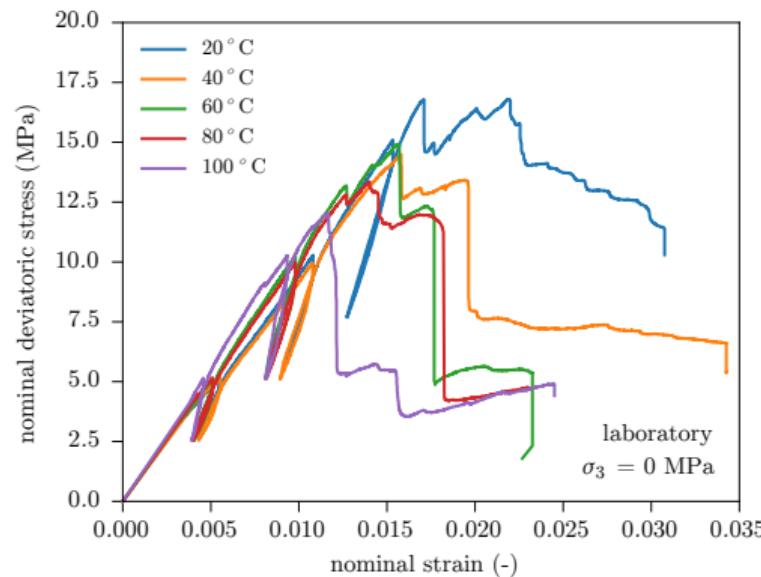
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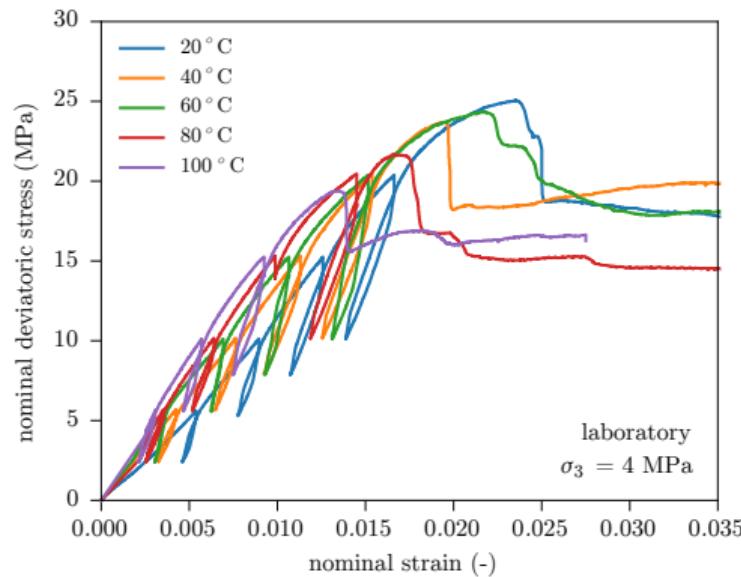
# Coupled THM BVP simulation

## Obtained results



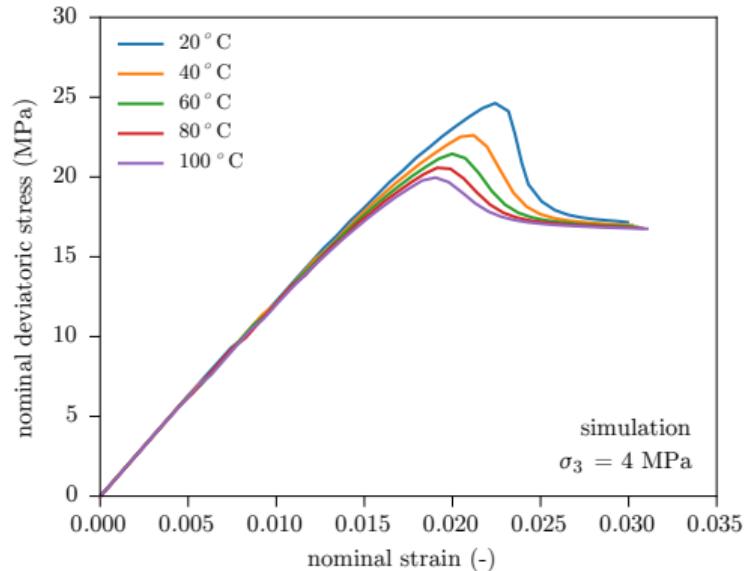
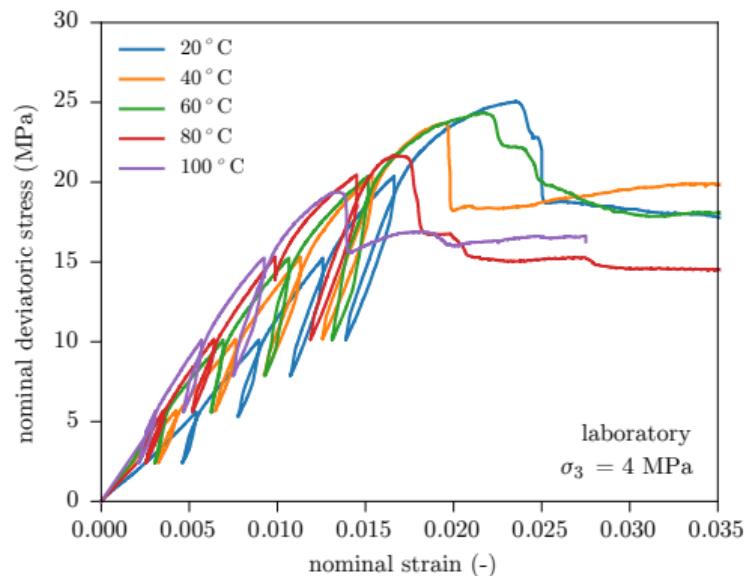
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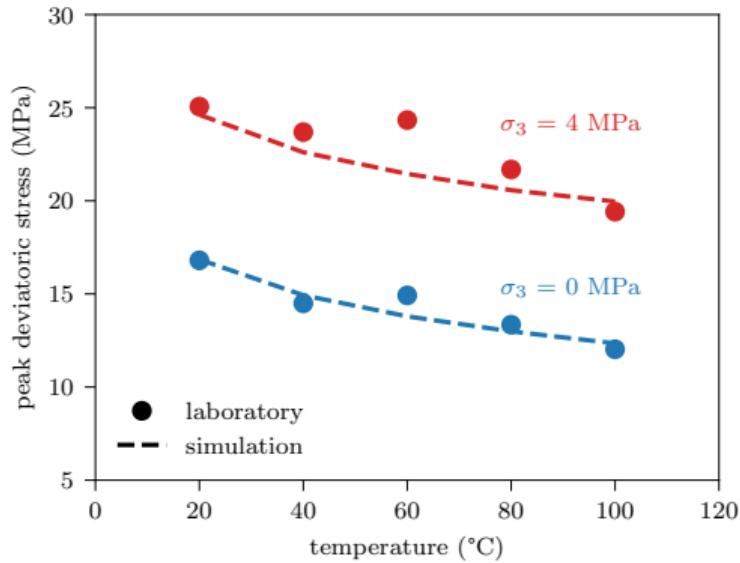
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# Content

## 1 Introduction

## 2 Implementation of thermal effects

- Volumetric yield function
- Temperature dependence of the **deviatoric** yield surface
- Temperature dependence of the **volumetric** yield surface
- Additional convergence checks

## 3 Coupled THM BVP simulation

## 4 Conclusions

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- Including the expansion-contraction transition observed as the temperature is increased in temperature-controlled constant stress tests.

¡Thank you for your  
attention!

# References

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