



# Mikro- und Meso-Mechanische Simulationen zum Verformungsverhalten von Tongesteinen

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## Content

### 1. General comments on micro-mechanical modelling

### 2. Micro- and meso-mechanical modelling of Opalinus Clay

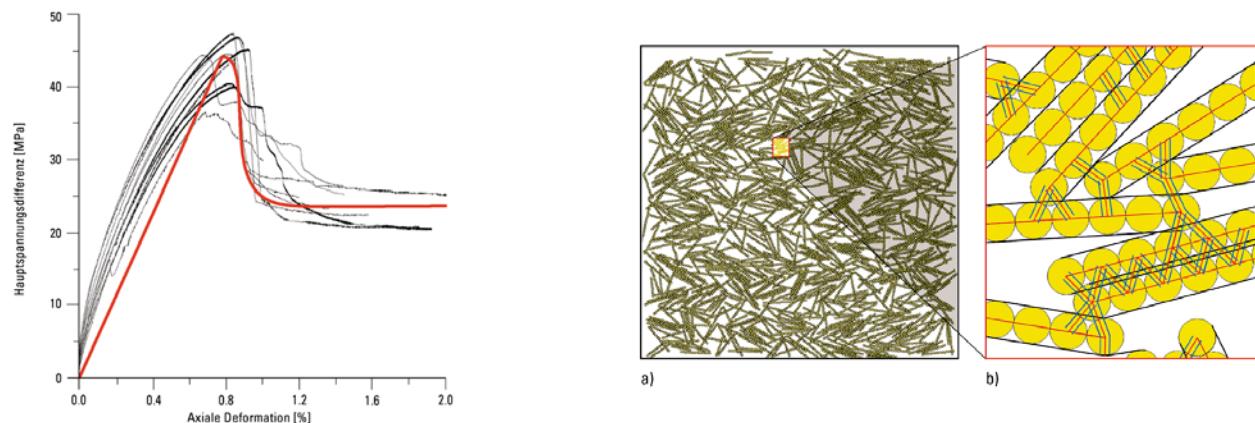


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## Method of approach

Macro-mechanical view  
(scale: dm, m, km)  
„Phenomenological“ concept

Micro-mechanical view  
(scale: nm,  $\mu$ m, mm)  
„Physical“ concept



# Micromechanical simulation approaches



# Choice of simulation approach

**deformable  
polyhedra**



Voronoi-bodies

- more physics, more flexible
- computer-intensiv
- potential of numerical instability

**stiff  
spheres**

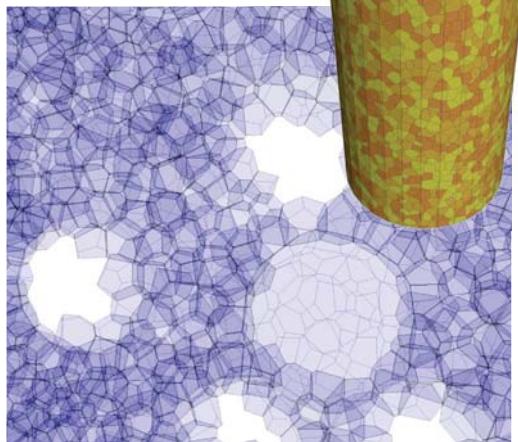
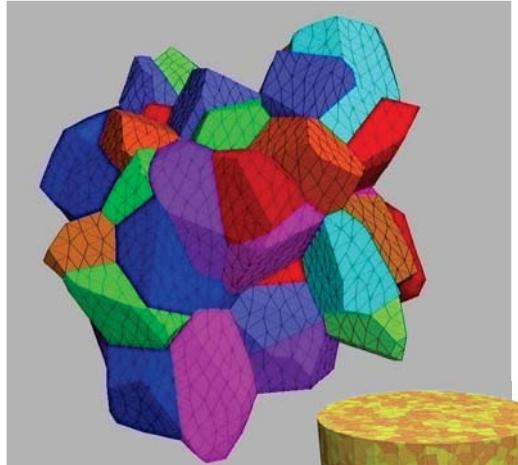


Spheres-Clusters-Clumps

- robust, fast, stable
- physical less flexible

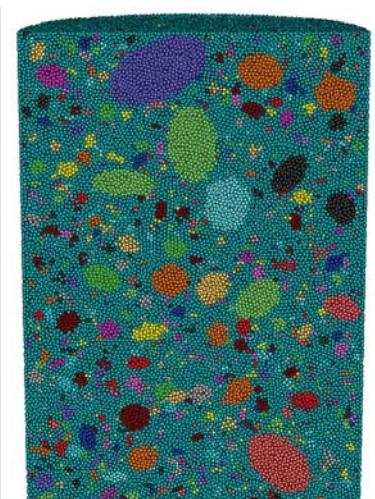
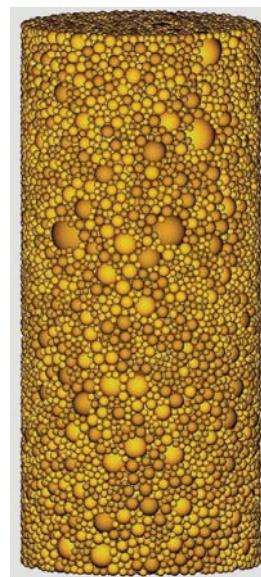
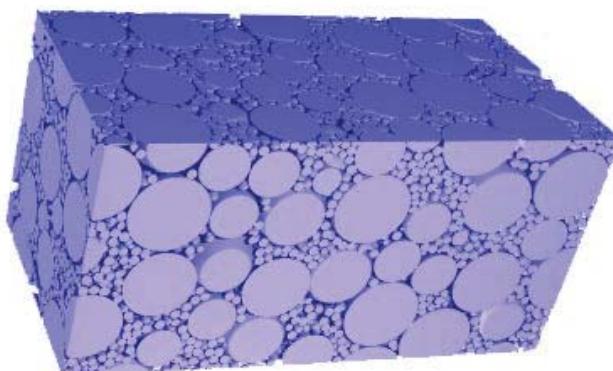
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## Generation of models



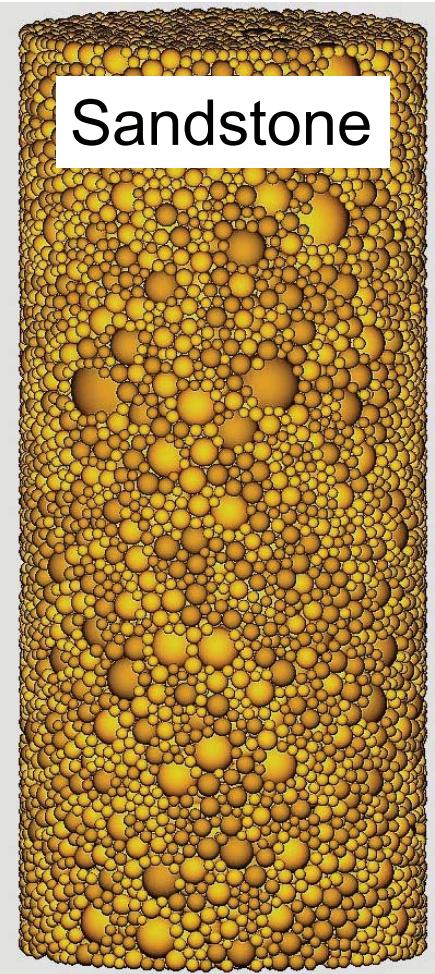
Voronoi Bodies

Spheres – Clumps - Clusters

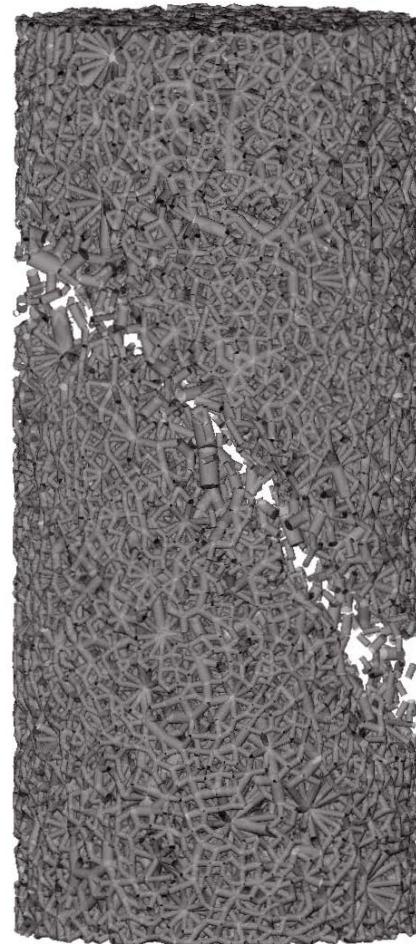


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Model set-up based on spheres  
according to grain size distribution



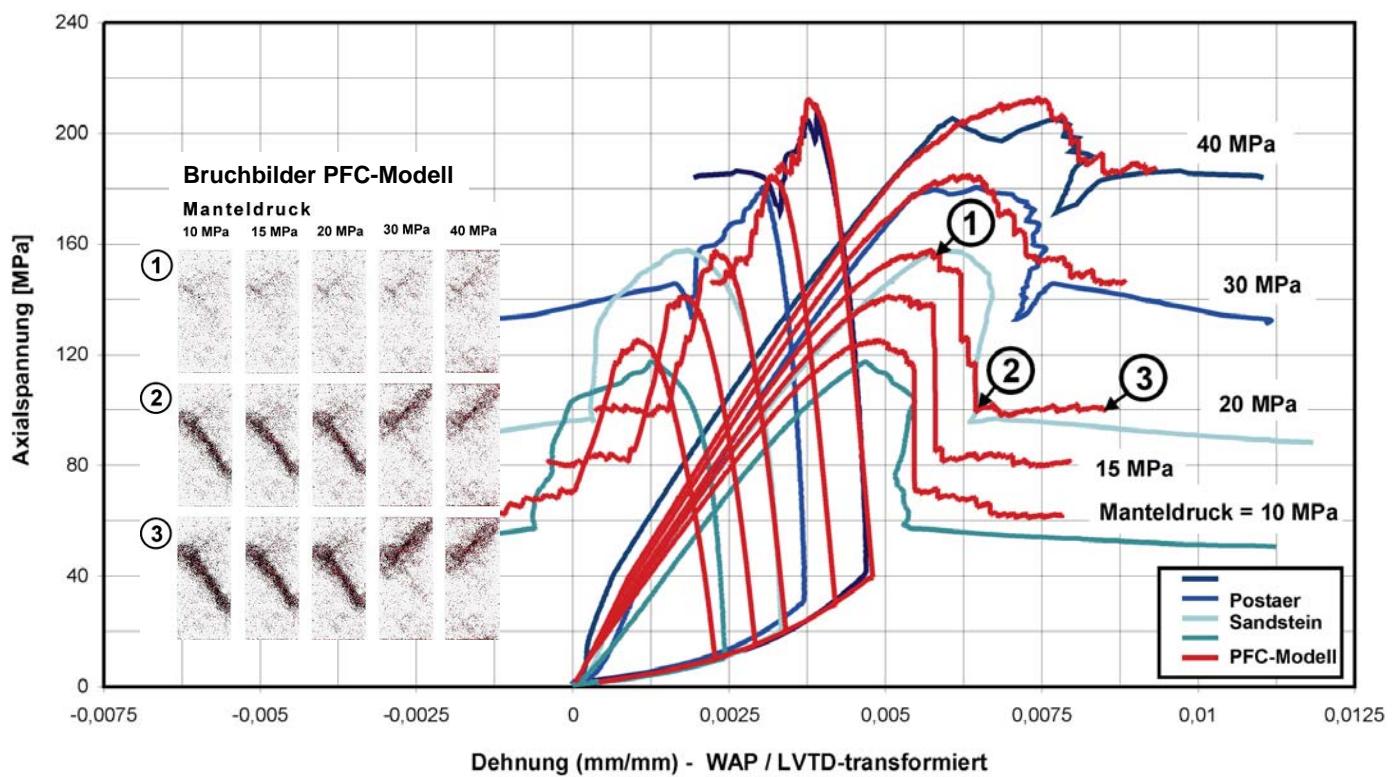
Shear fracture during triaxial testing



Baumgarten & Konietzky 2013

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Sandstone

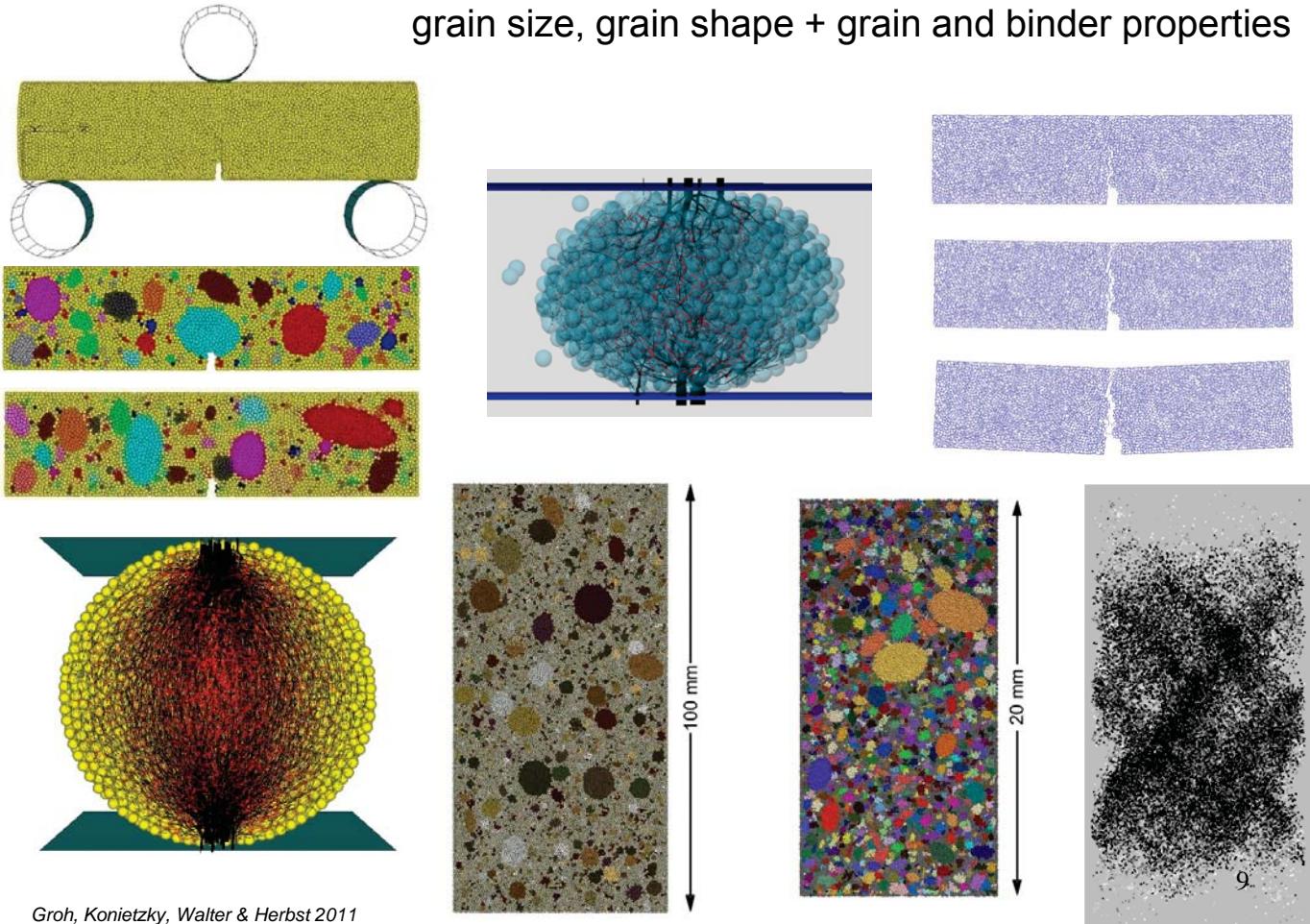


Longitudinal deformation and transverse deformation  
including hydrostatic pre-loading

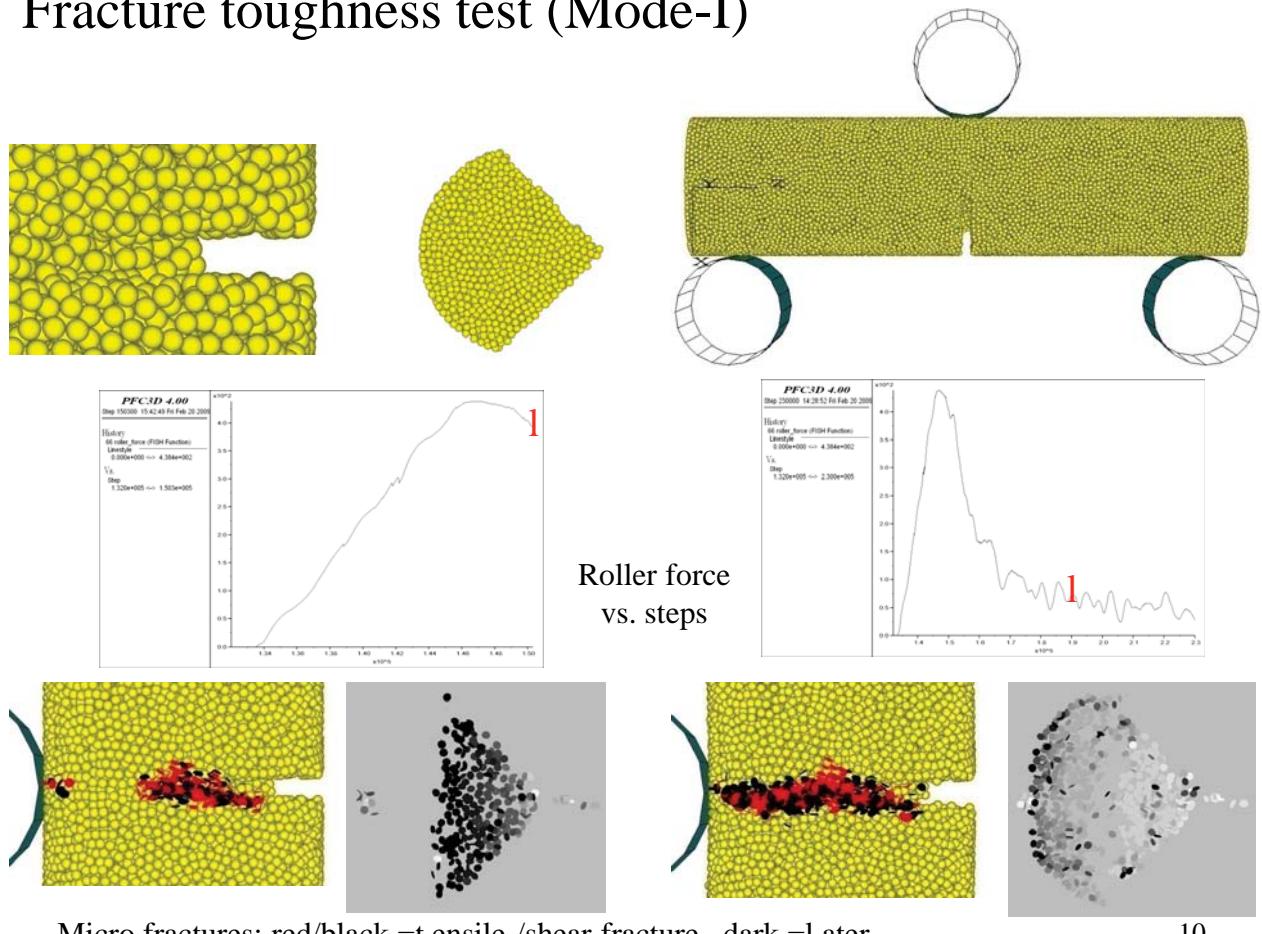
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Baumgarten & Konietzky 2013

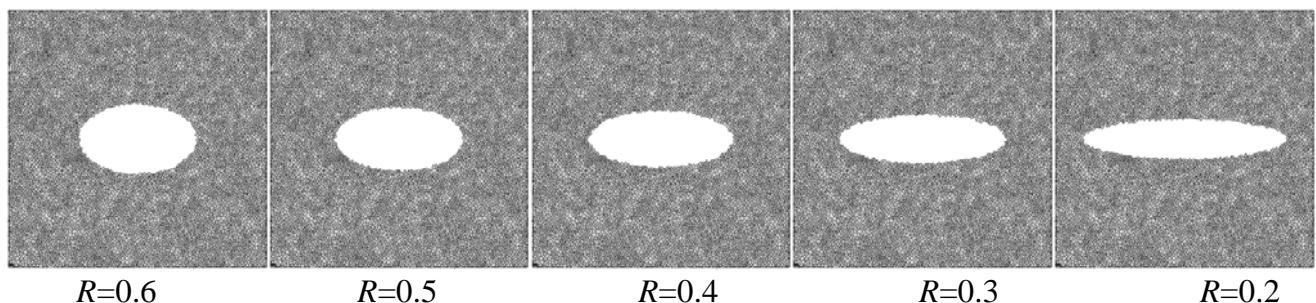
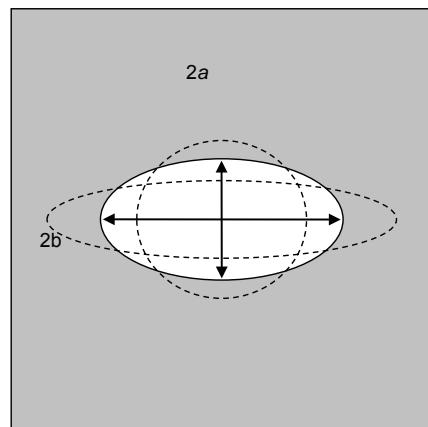
# Micromechanical simulation of concrete considering grain size, grain shape + grain and binder properties



## Fracture toughness test (Mode-I)



# Micro-mechanical model of single pore of different shape

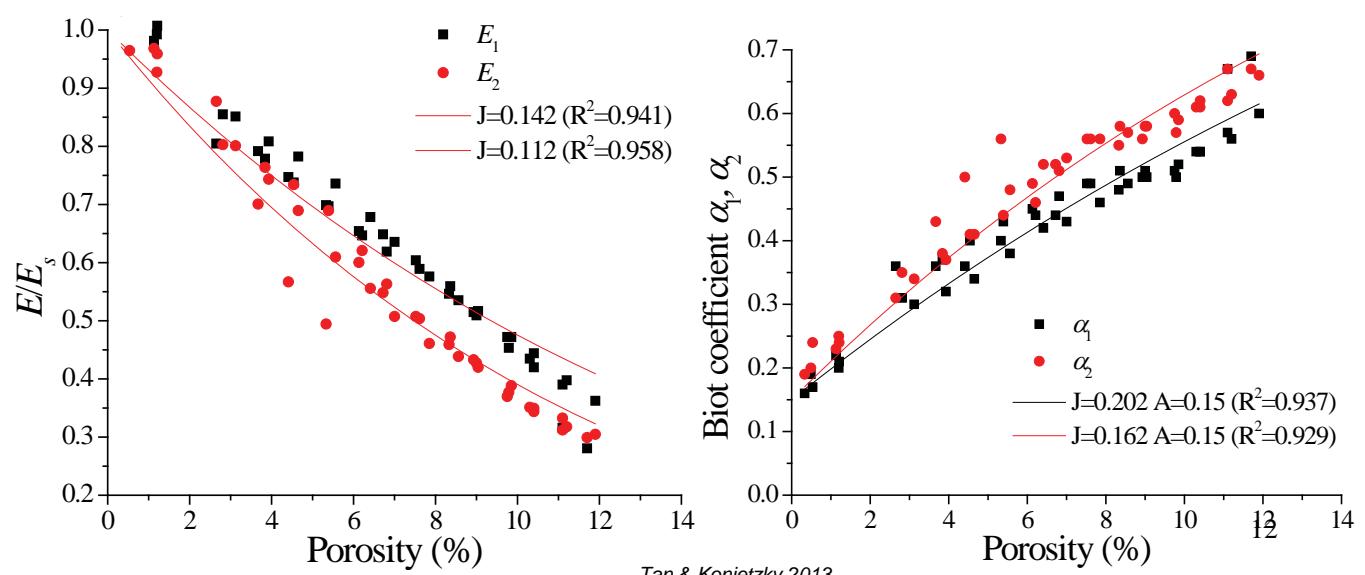
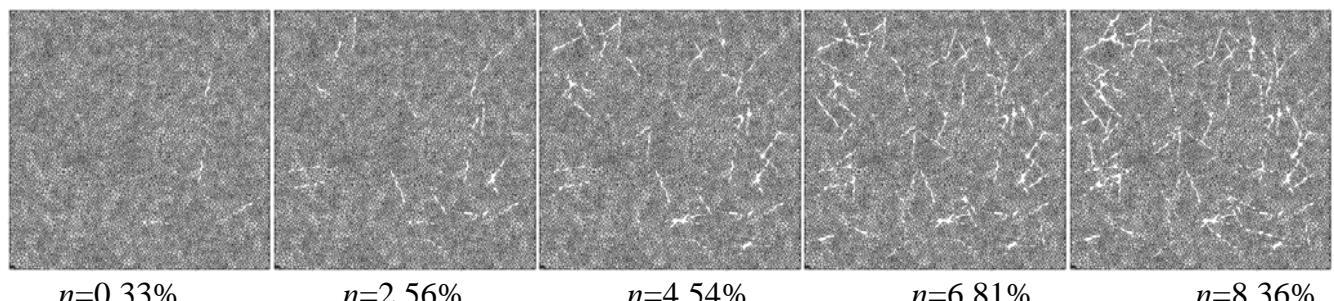


Elliptical pores with different aspect ratio

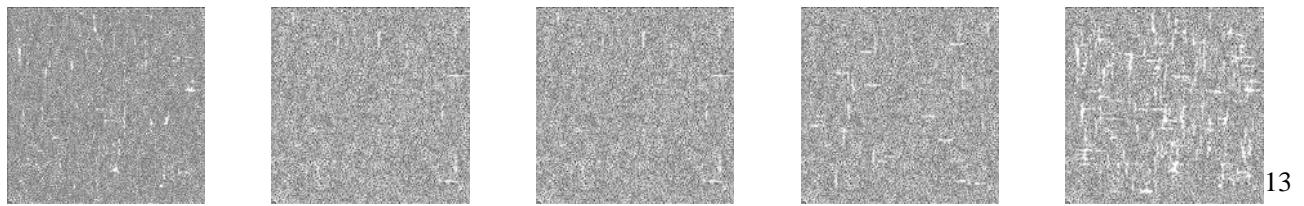
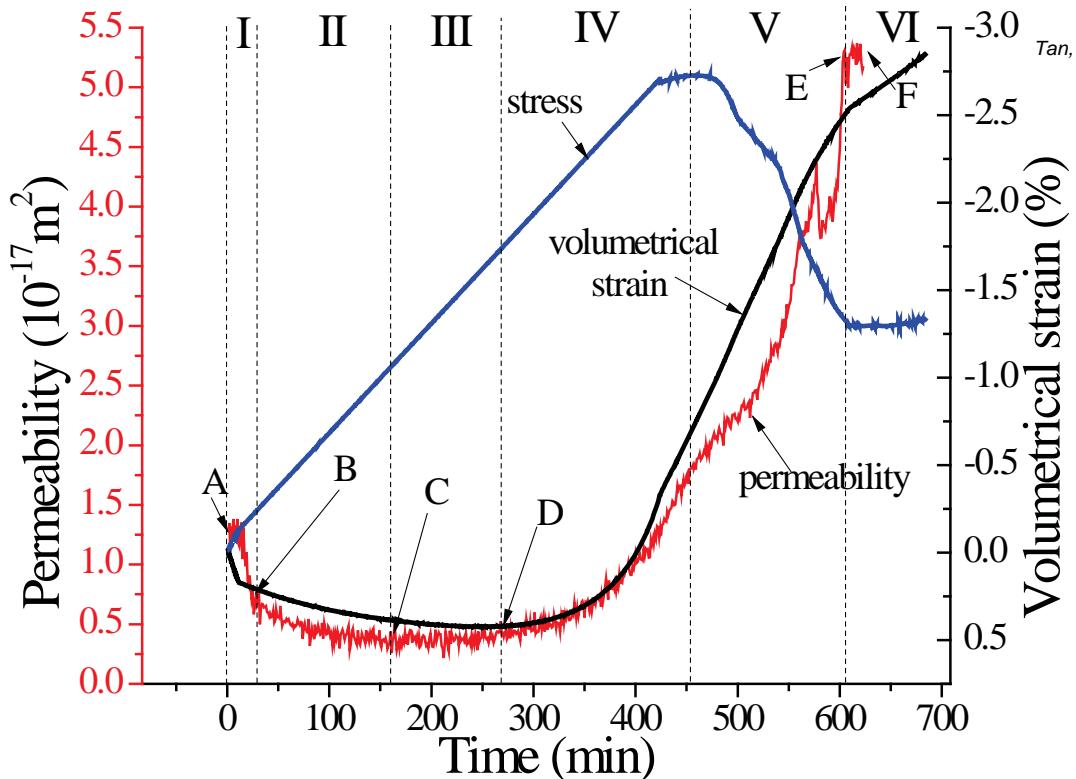
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Tan & Konietzky 2013

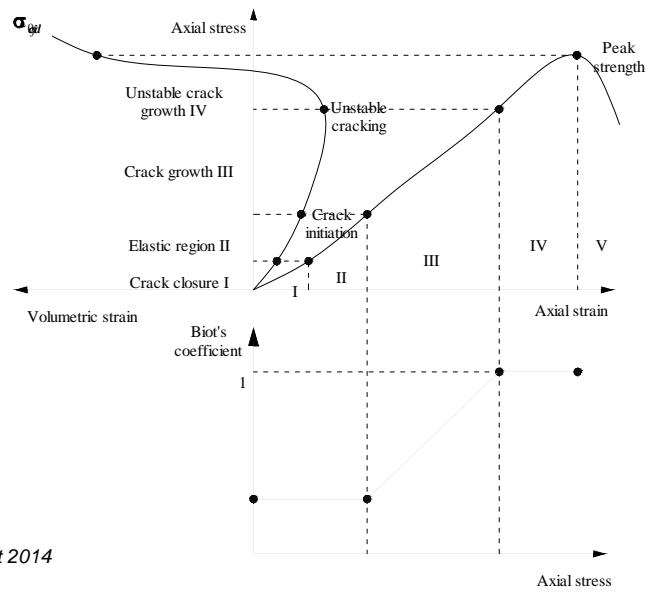
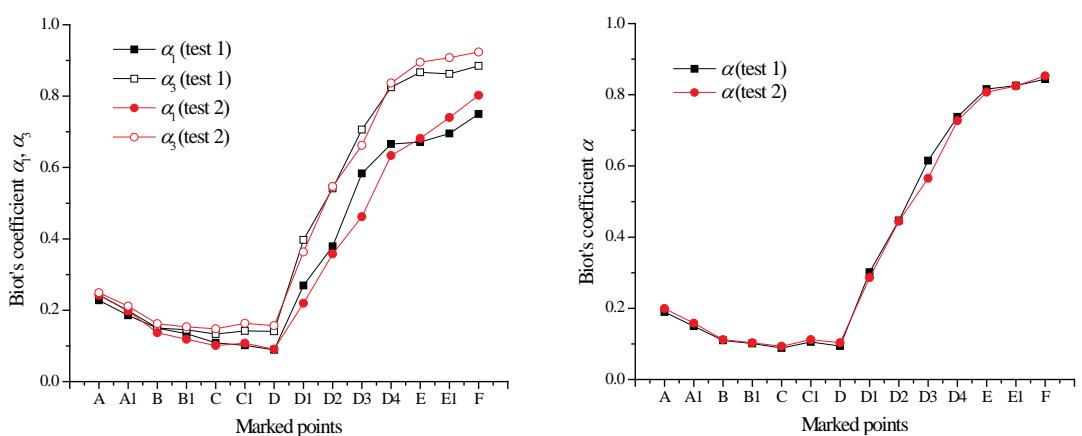
## Random elliptical cracks ( $S=0.1$ )



Tan & Konietzky 2013

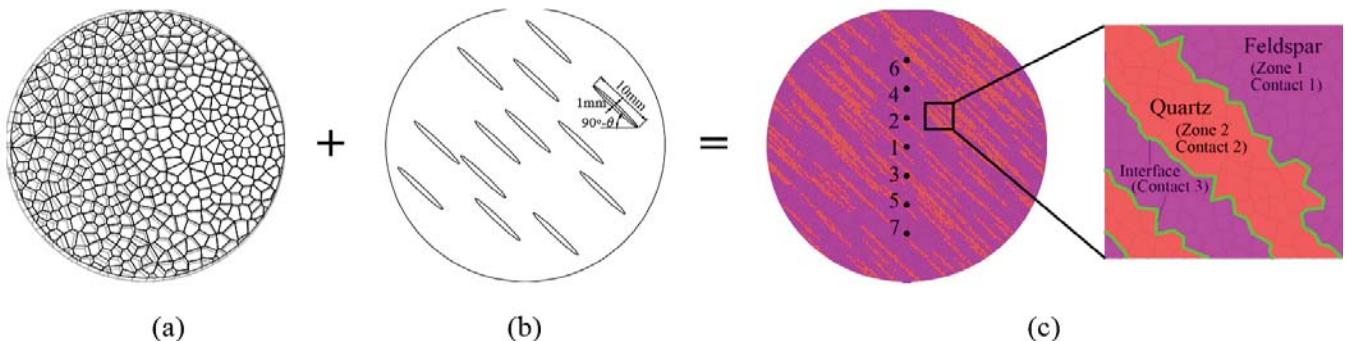
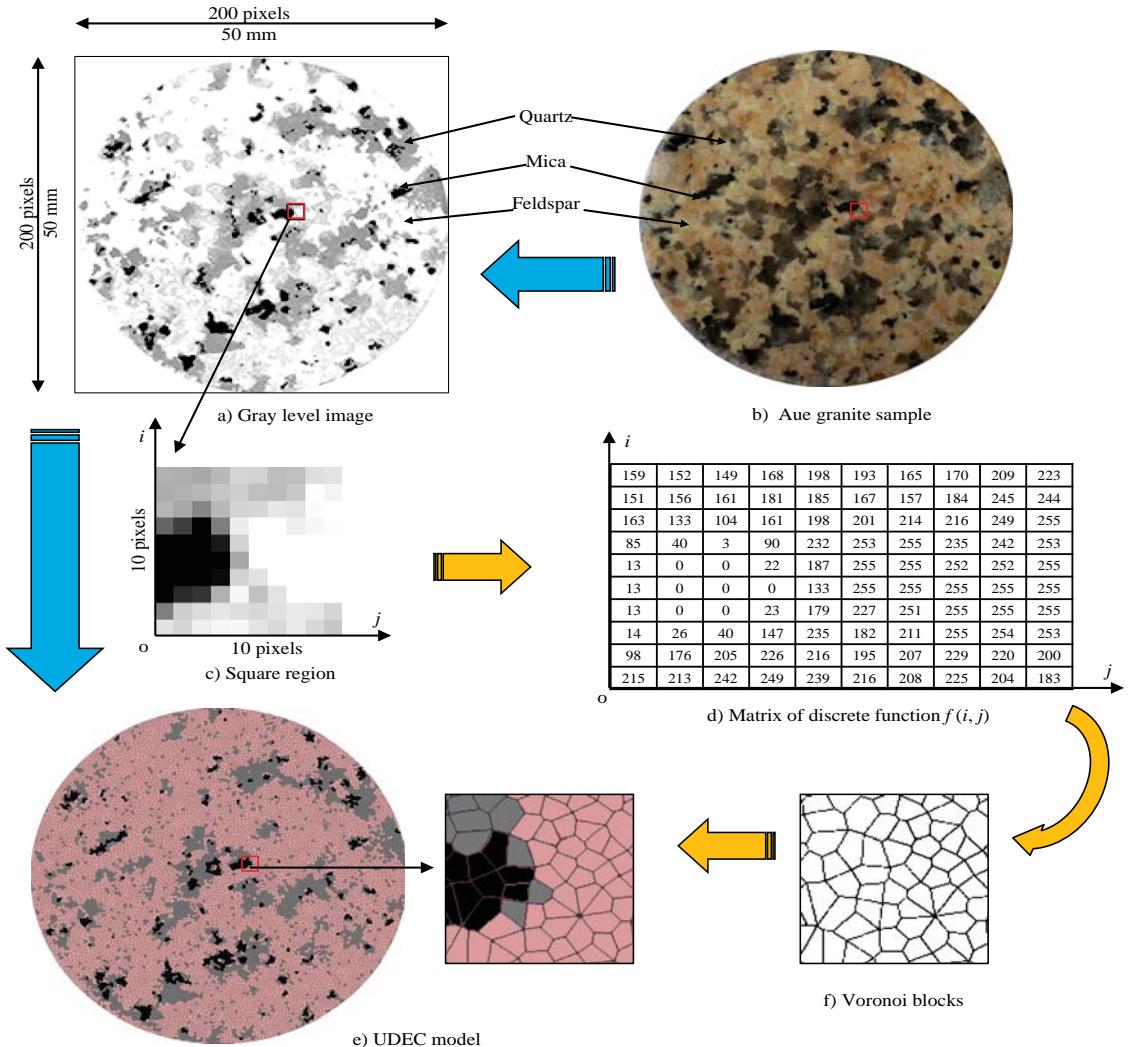


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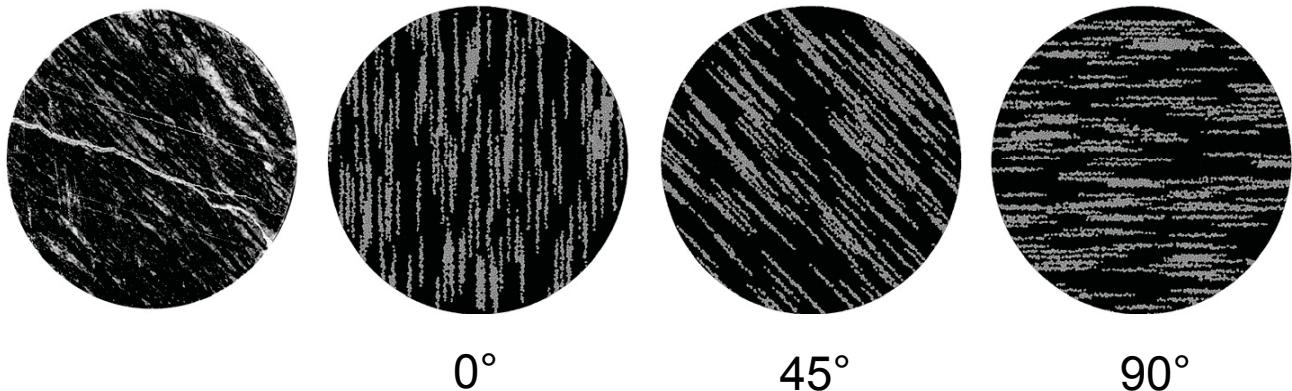


## Gray level image technique to duplicate microstructure

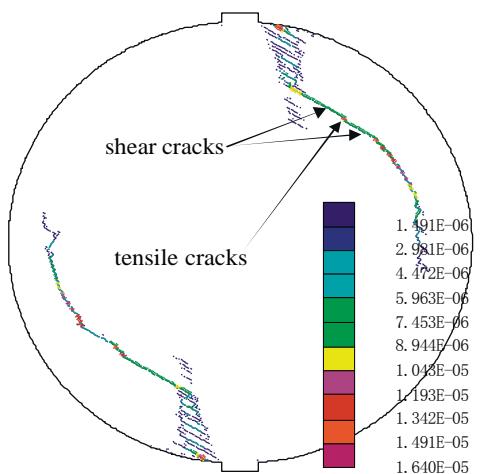
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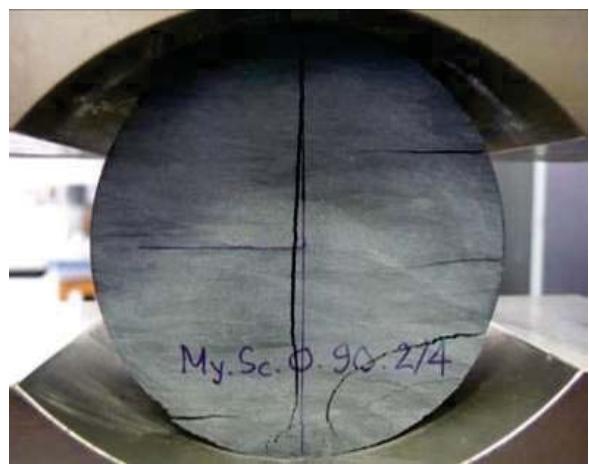
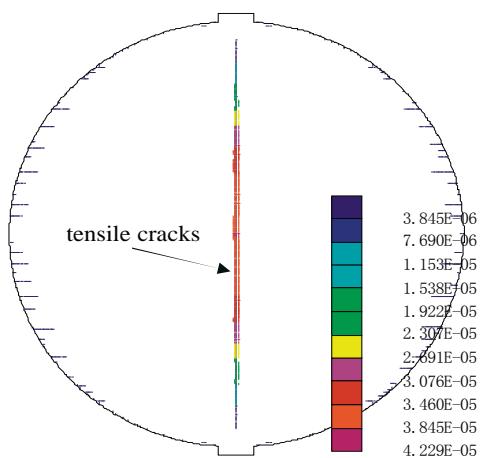
Micro-structural model of gneiss disc



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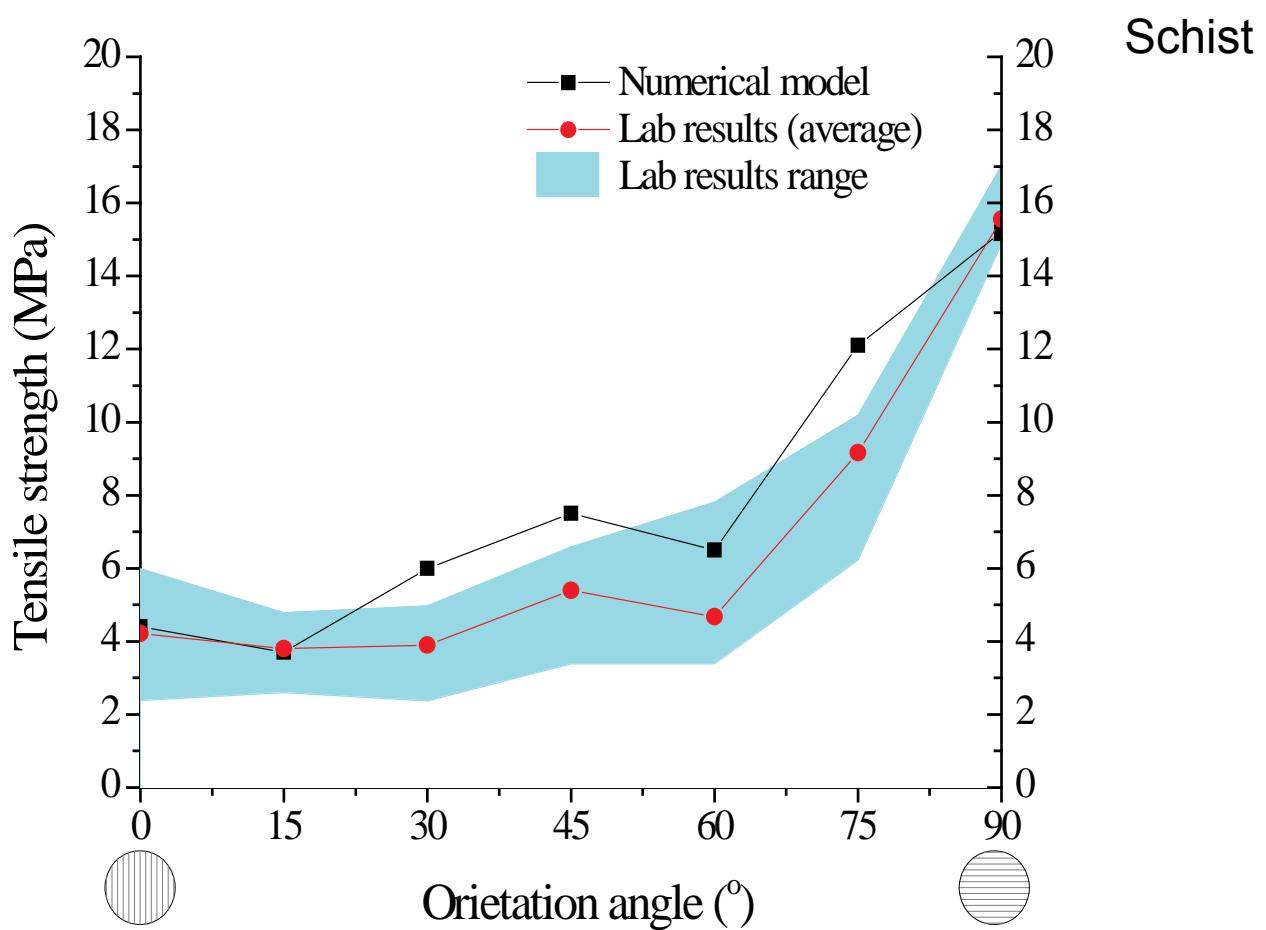


60°

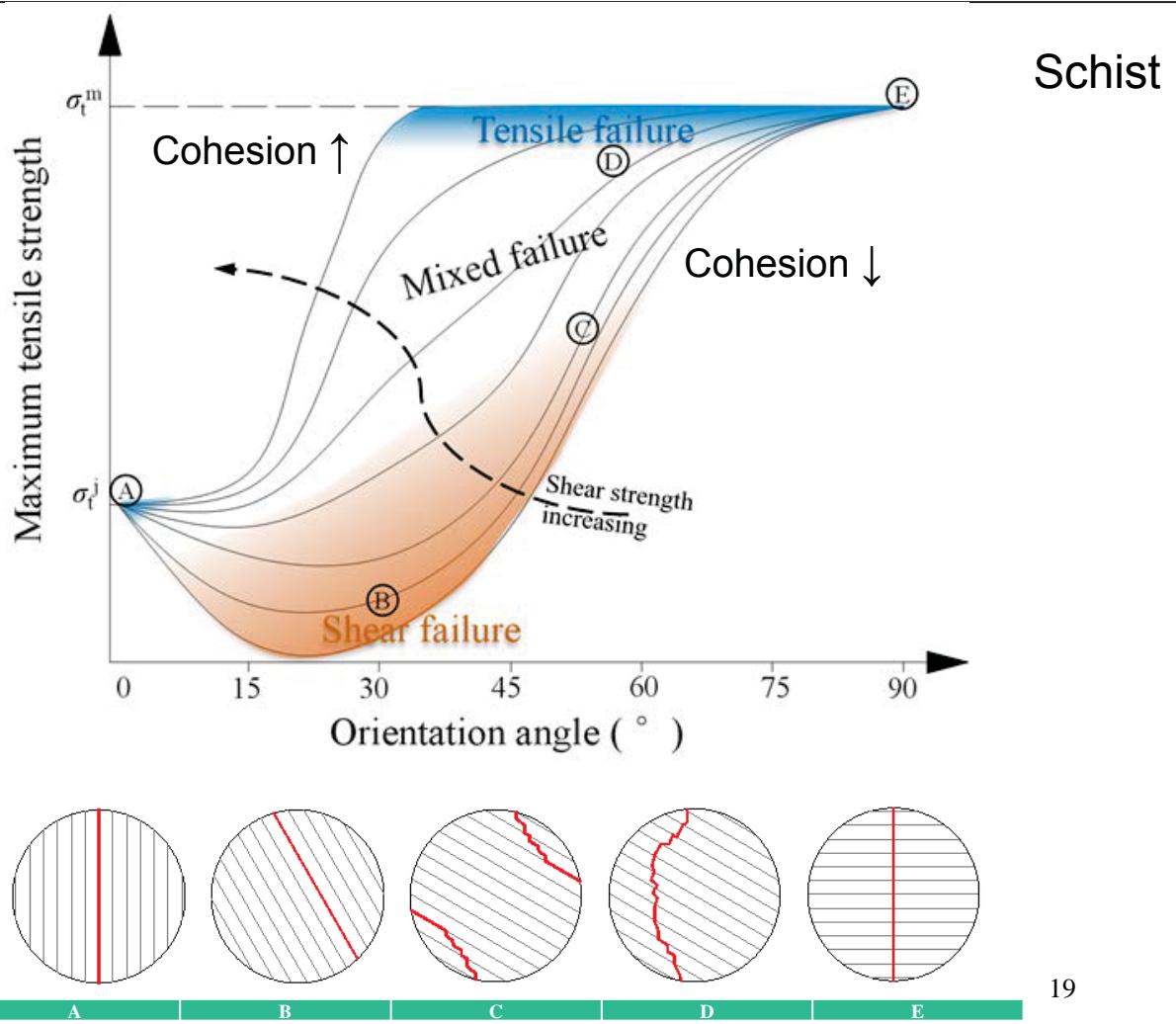


90°

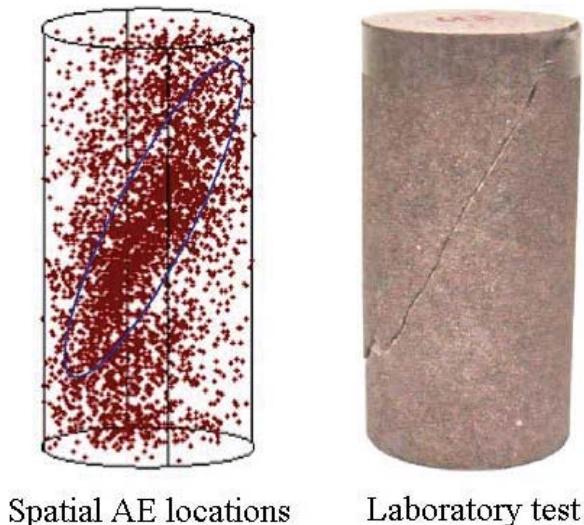
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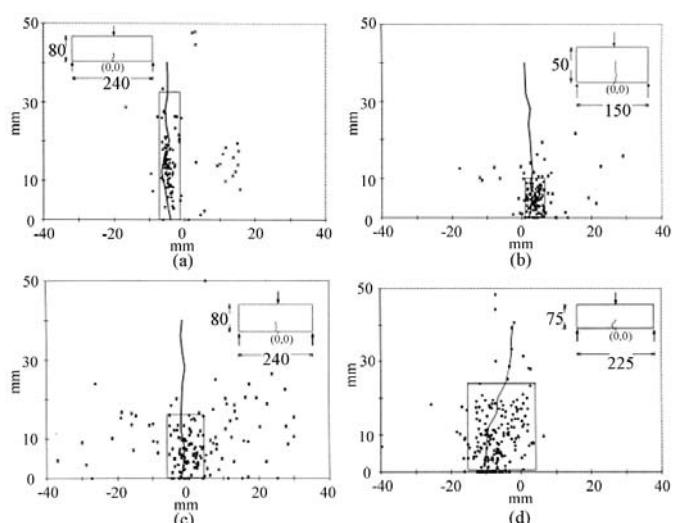
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## Lab test results



Spatial acoustic emission (AE) locations and experimental failure of red sandstone at a confining pressure of 35 MPa (Yang et al. 2012)



Acoustic emission (AE) locations and final macroscopic fracture pattern in the three-point bending test (a) Berea sandstone; (b) Sioux quartzite; (c) Charcoal granite; (d) Rockville granite (Zietlow and Labuz 1998)

# Theories and approaches utilized

Linear elastic fracture mechanics

Stress intensity factor approach

Subcritical crack growth theory

Charles equation

Crack propagation schemes

Elasto-plastic stress redistribution

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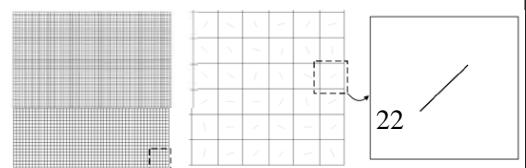
Subcritical crack growth simulation  
using Charles equation and cellular  
automate

$$t_{zone} = \int_{c_0}^{c_c} \frac{dc}{v}$$

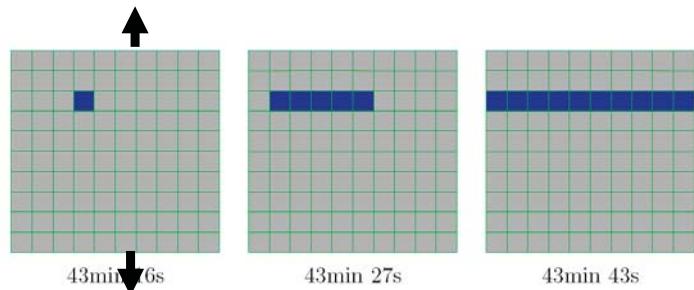
$$c_c = \min \{c_{Ic}, c_{IIc}, d_{zone}\} = \min \left\{ \frac{2}{\pi} \left( \frac{K_{Ic}}{\sigma} \right)^2, \frac{2}{\pi} \left( \frac{K_{IIc}}{\tau} \right)^2, d_{zone} \right\}$$

$$t_{zone} = \int_{c_0}^{c_c} [v(K_I) + v(K_{II})]^{-1} dc = \int_{c_0}^{c_c} [AK_I^n + AK_{II}^n]^{-1} dc$$

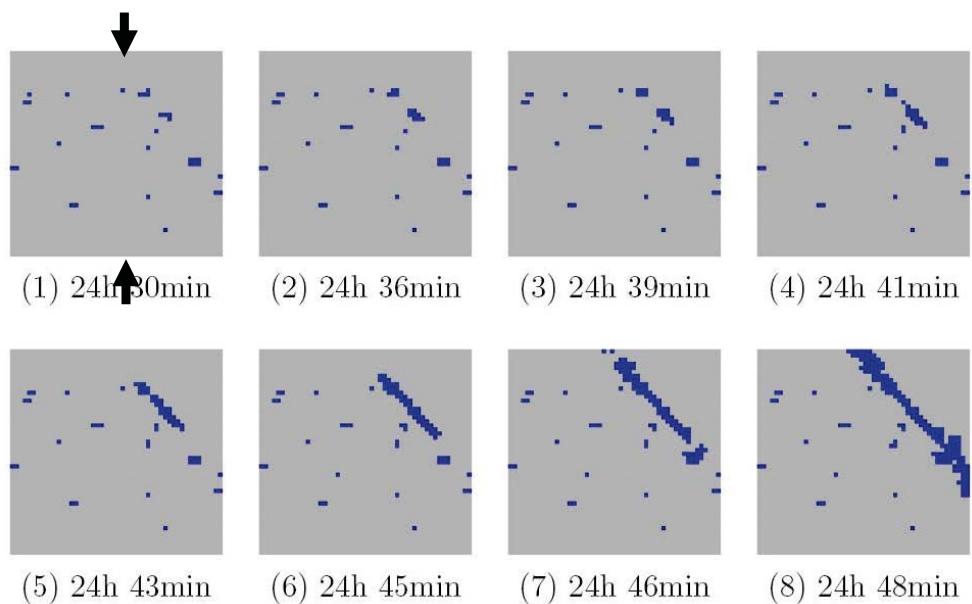
$$\begin{aligned} t_{zone} &= \frac{1}{A} \int_{c_0}^{c_c} \left[ \left( \sigma \left( \frac{1}{2} \pi c \right)^{1/2} \right)^n + \left( \tau \left( \frac{1}{2} \pi c \right)^{1/2} \right)^n \right]^{-1} dc \\ &= \frac{1}{A (\sigma^n + \tau^n)} \left( \frac{2}{\pi} \right)^{n/2} \int_{c_0}^{c_c} c^{-n/2} dc \\ &= \frac{1}{A (\sigma^n + \tau^n)} \left( \frac{2}{\pi} \right)^{n/2} \frac{c_c^{1-n/2} - c_0^{1-n/2}}{1 - n/2} \end{aligned}$$



uniaxial  
tension



uniaxial  
compression

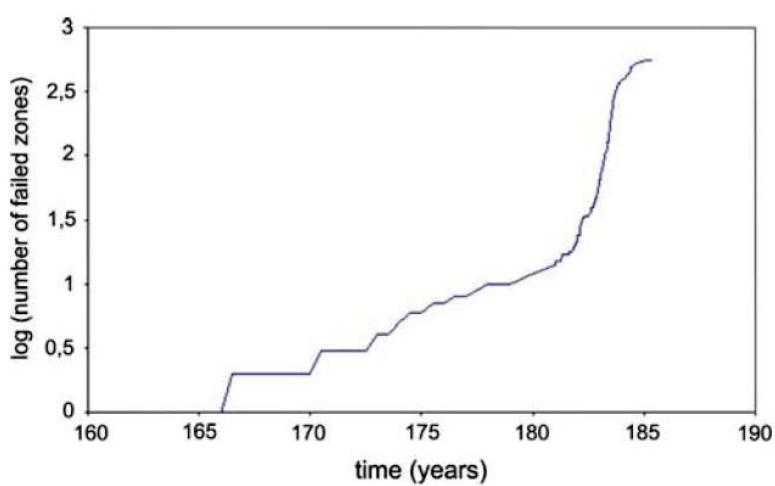


## Typical damage development during uniaxial loading

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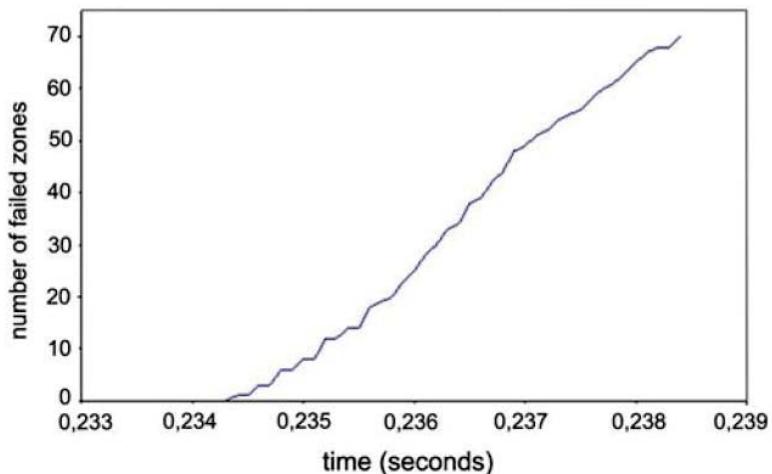
Konietzky, Heftenberger & Feige 2009

Comparison: damage development  
under uniaxial compression and tension



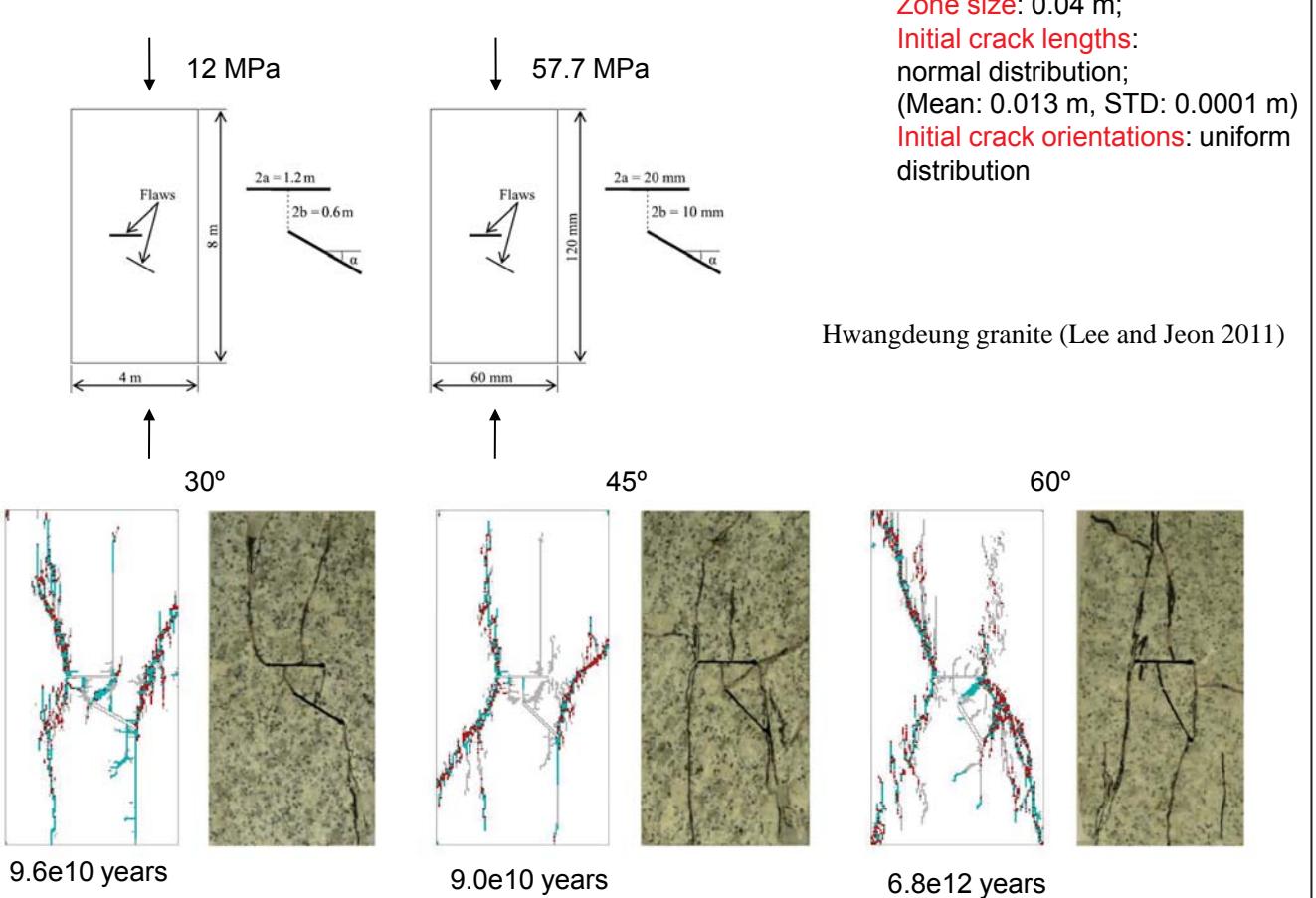
Compressive load

Same load  
magnitude !!



Tensile load

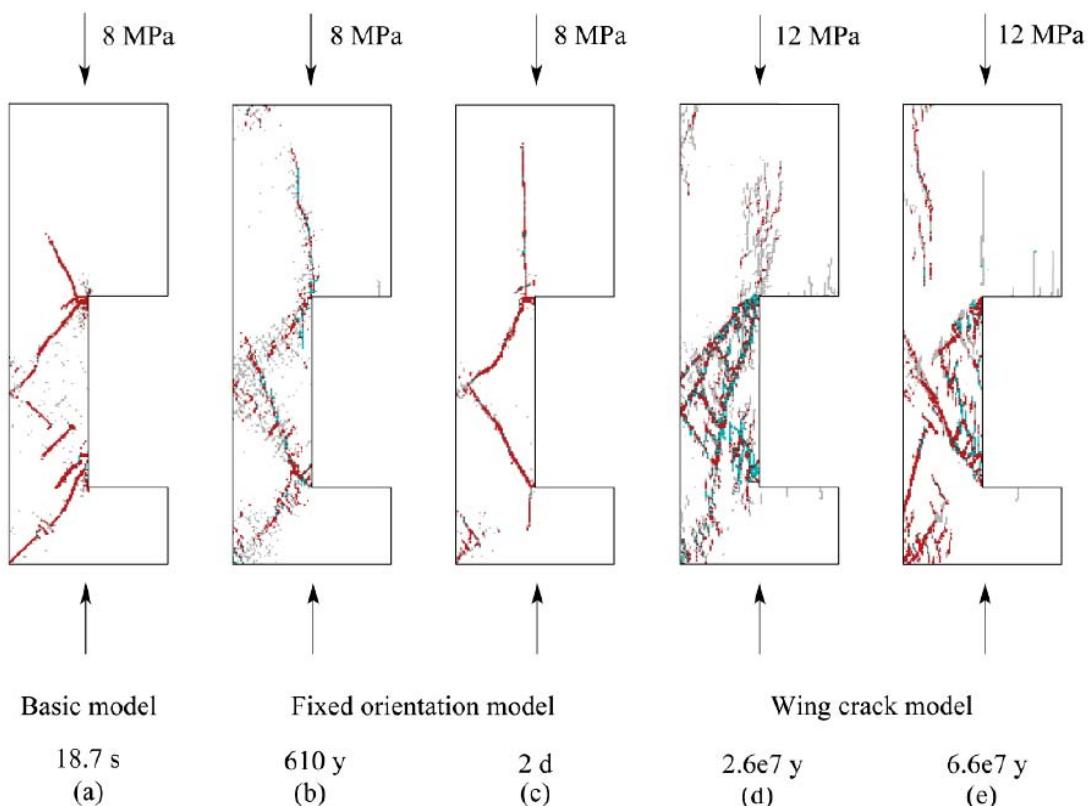
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Li & Konietzky 2013

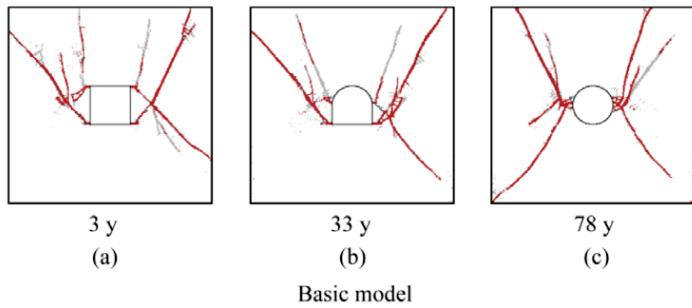
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## Practical Application: Pillar

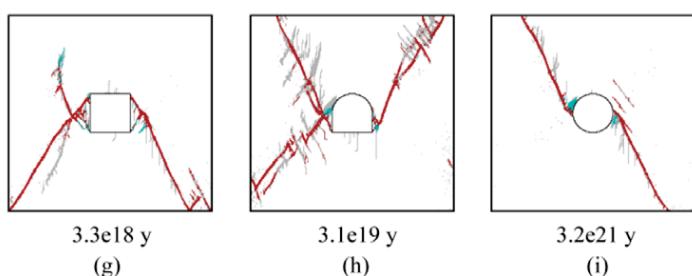
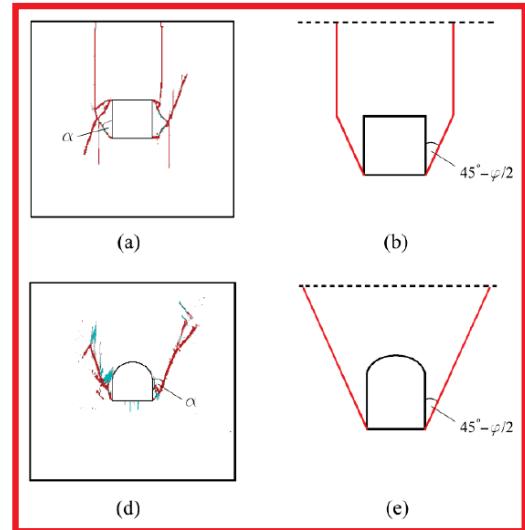
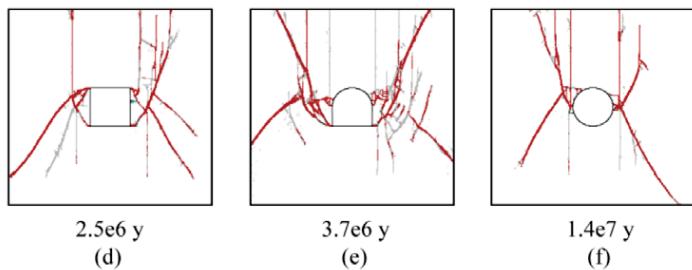


Li & Konietzky 2013

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## Practical Application: Tunnel , Drift



*Li & Konietzky 2013*

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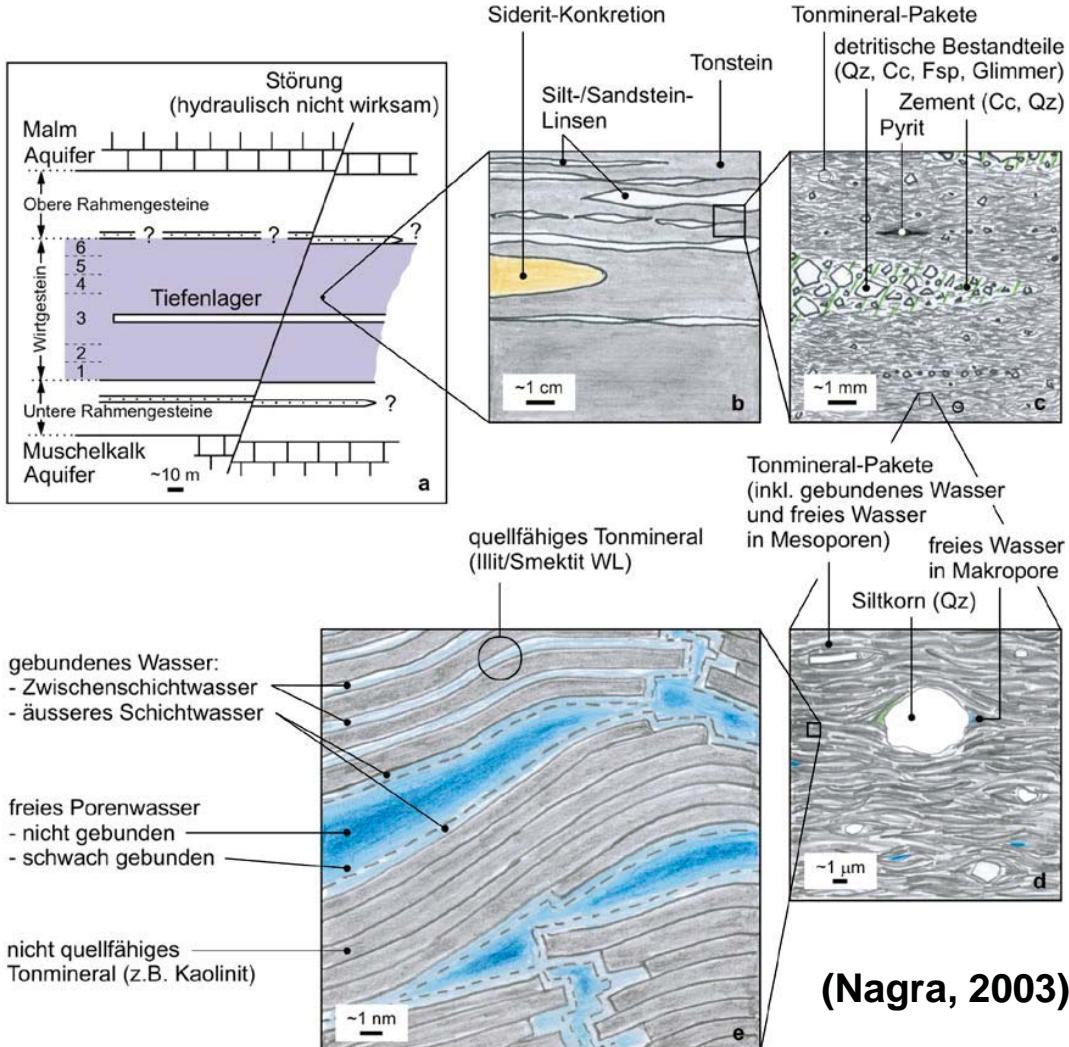
# Model concepts

for

# Opalinus clay



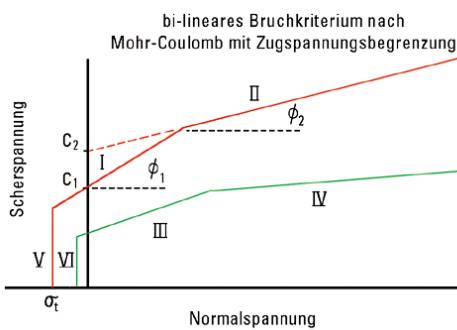
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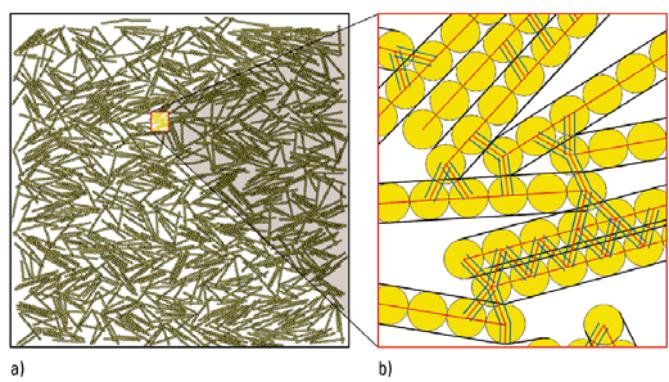
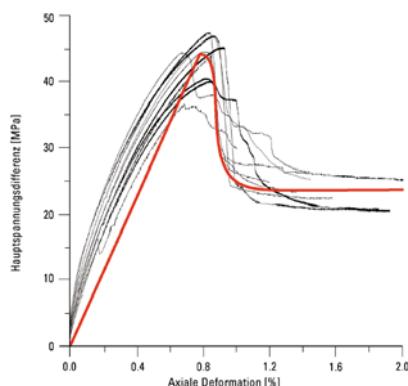
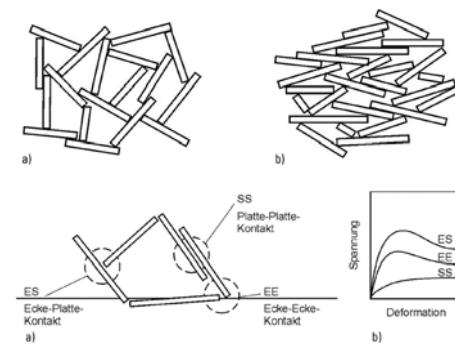
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## 2 concepts

„Phenomenological“  
concept



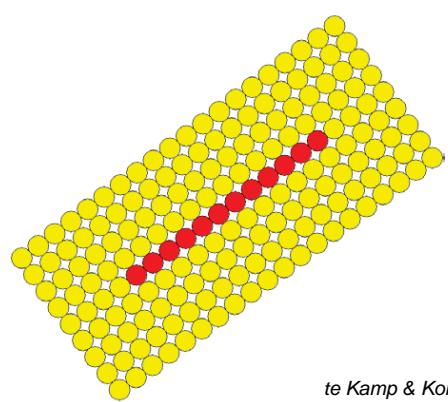
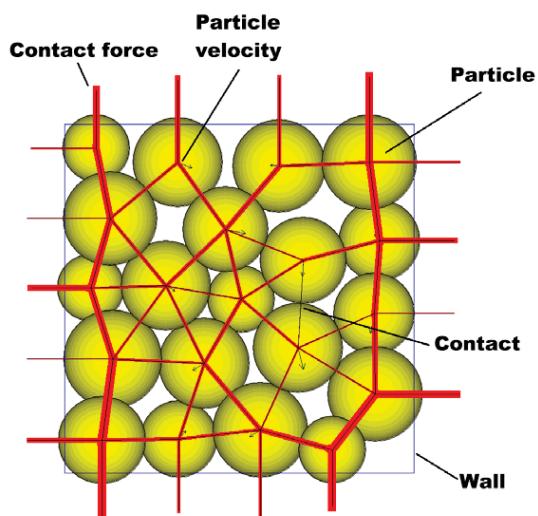
„Physical“ concept



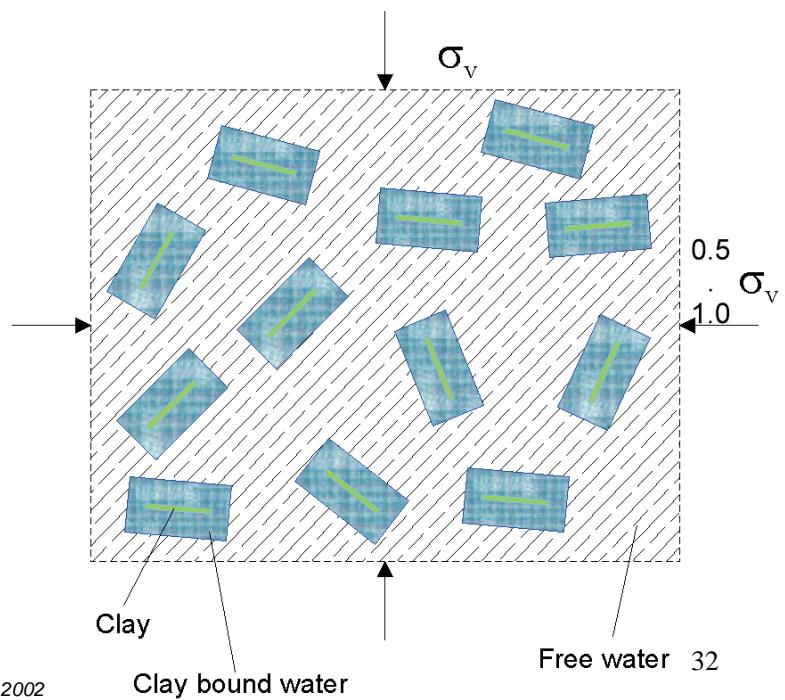
# „Physical“ concept at the micro-scale

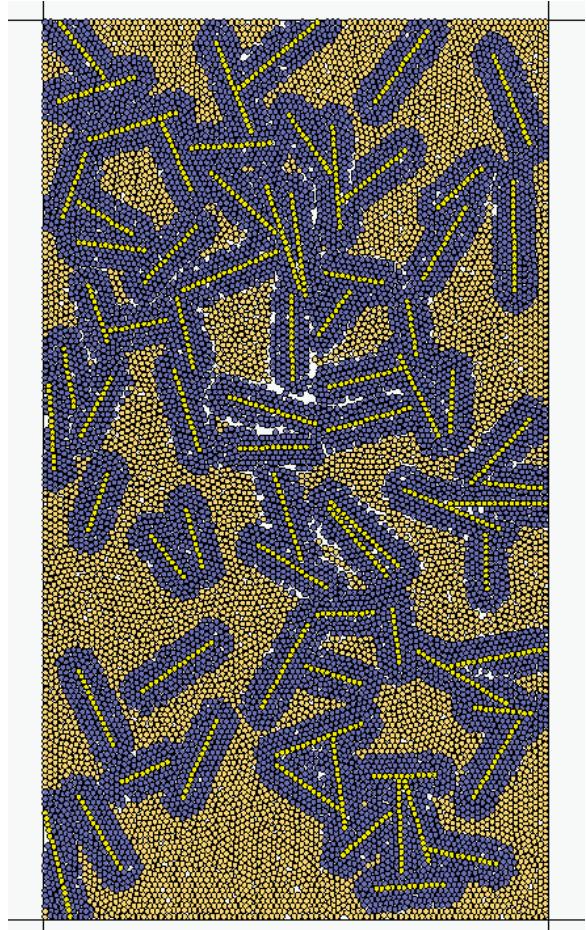


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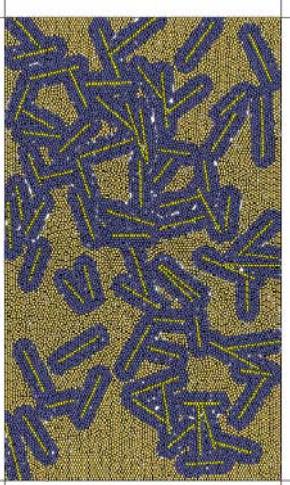
Numerical model  
with clay plates, free water and  
bounded water  
(Lennard-Jones-Potential)



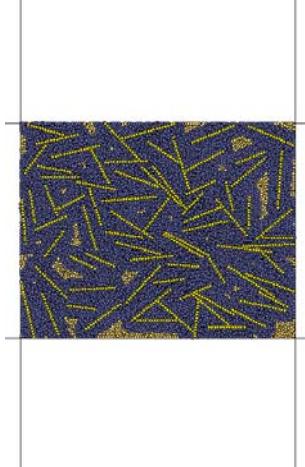


Model set-up

Initial state



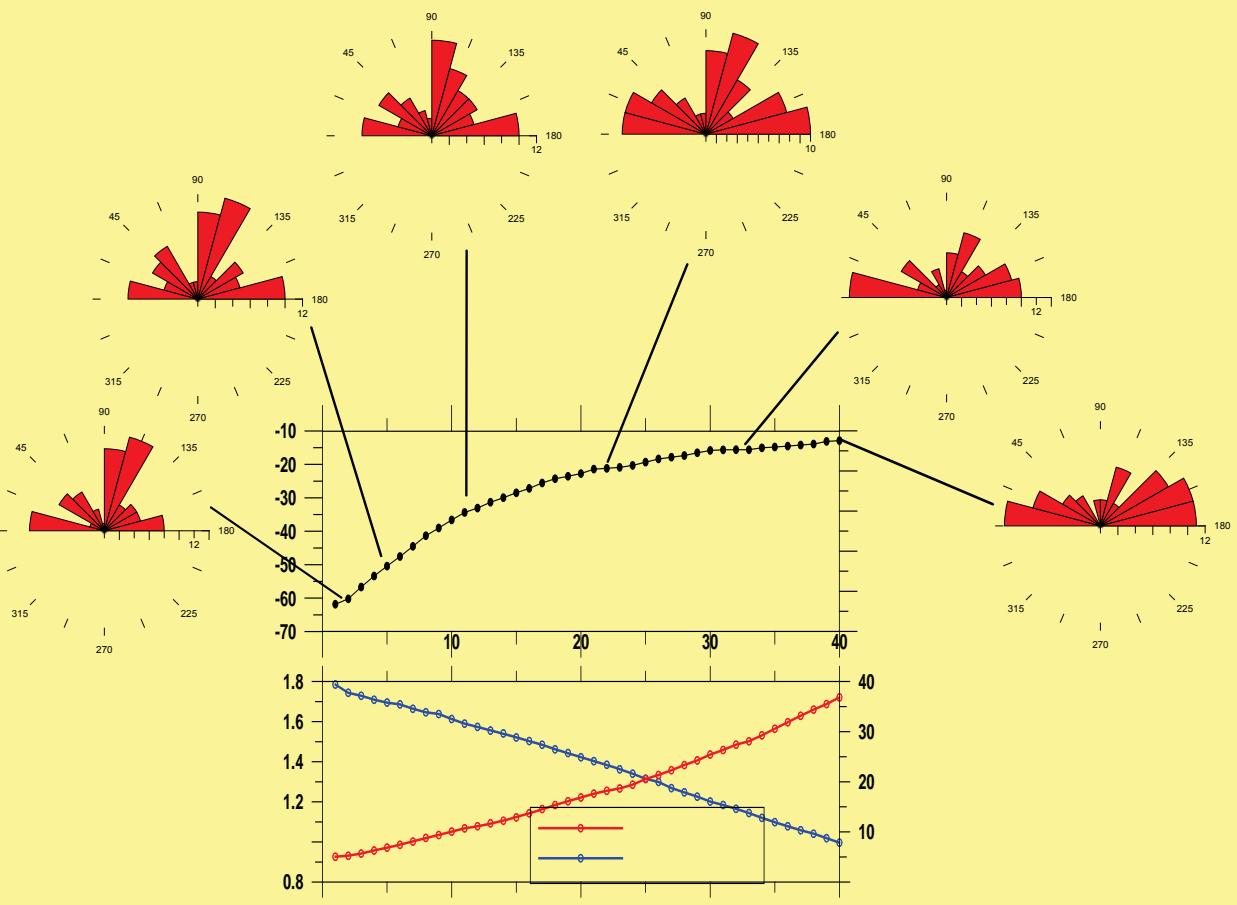
Final state



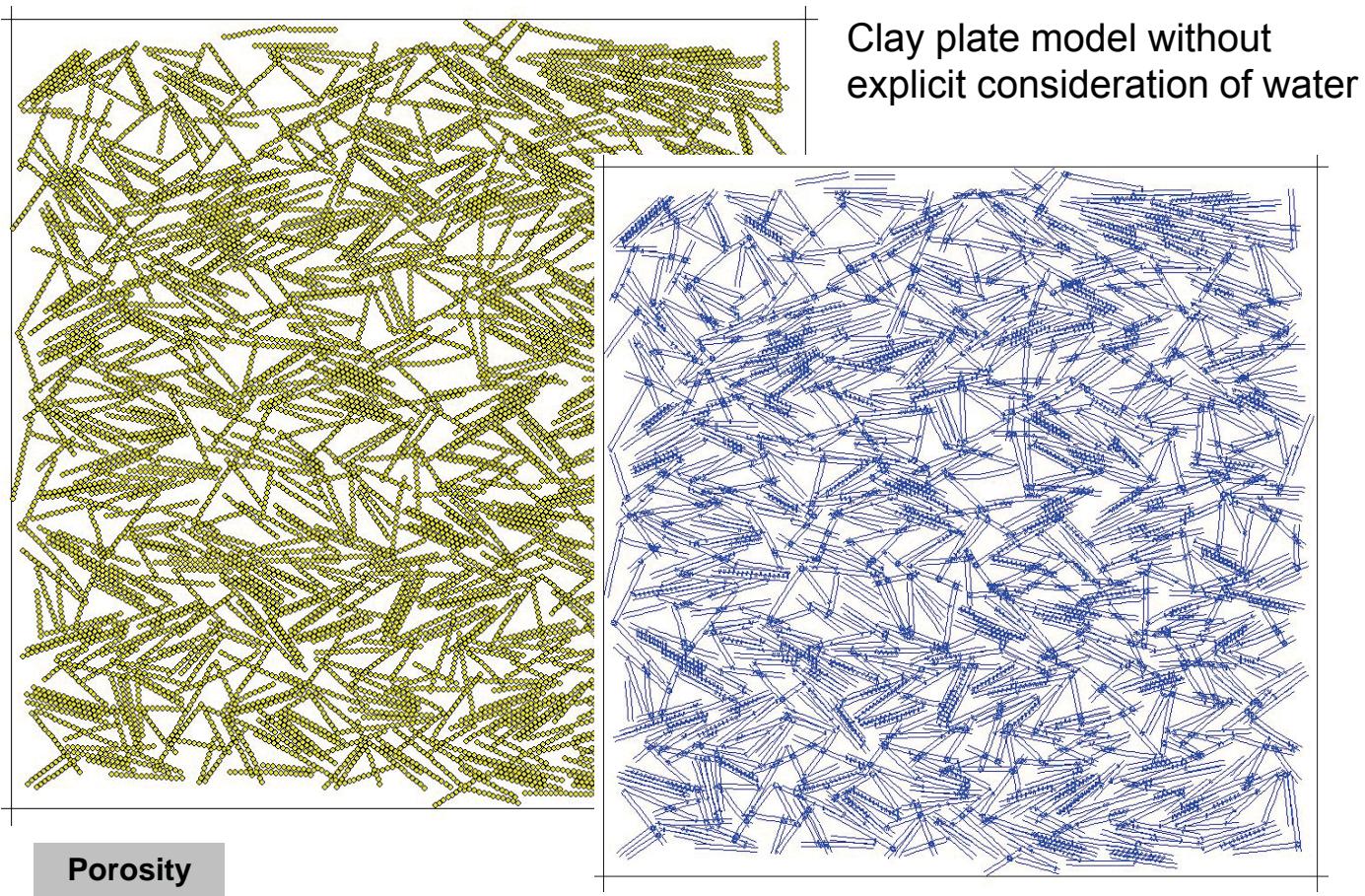
Compaction of  
saturated clay package  
under loading

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## Re-orientation of clay plates during compaction process

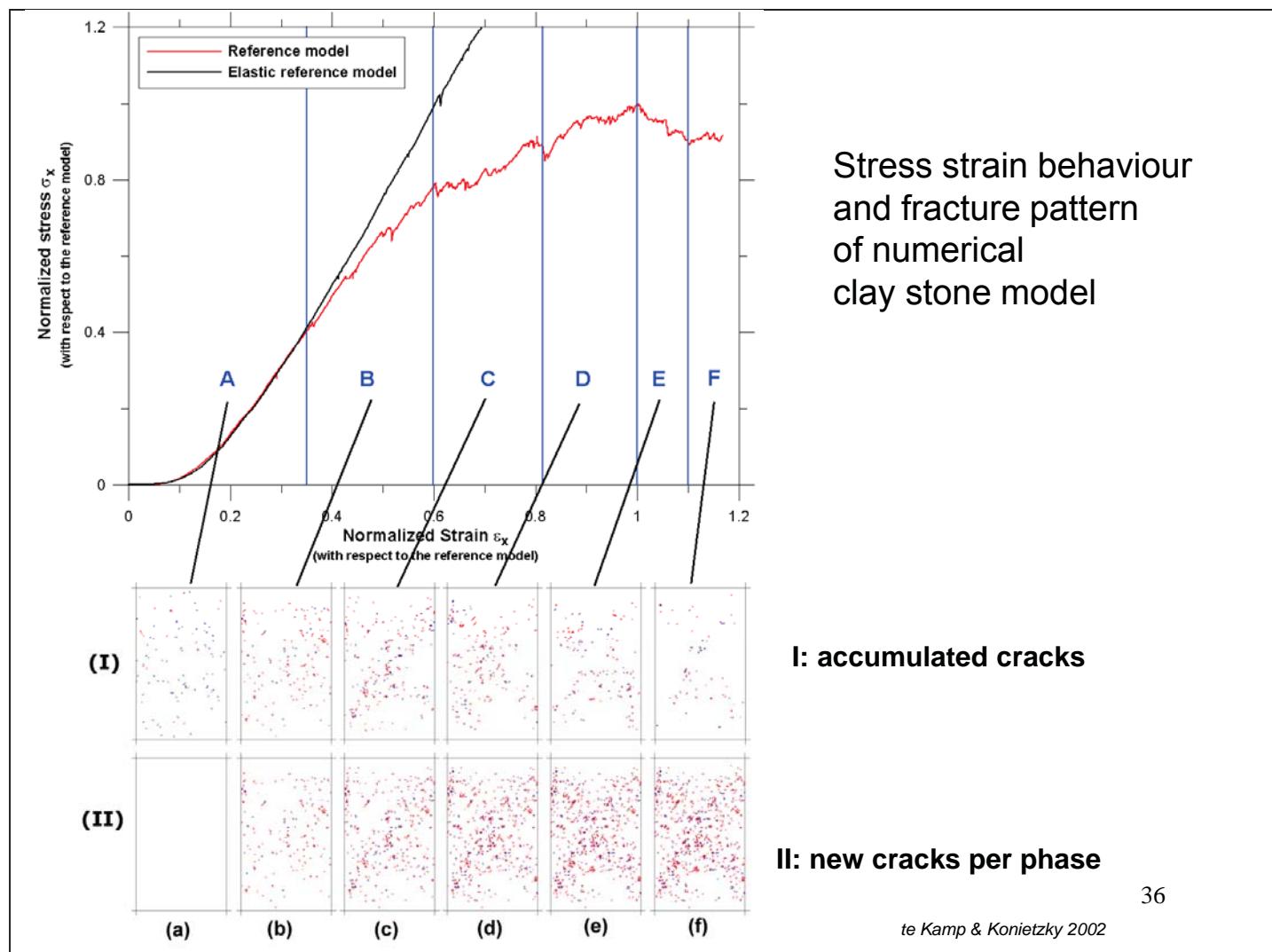


te Kamp & Konietzky 2002

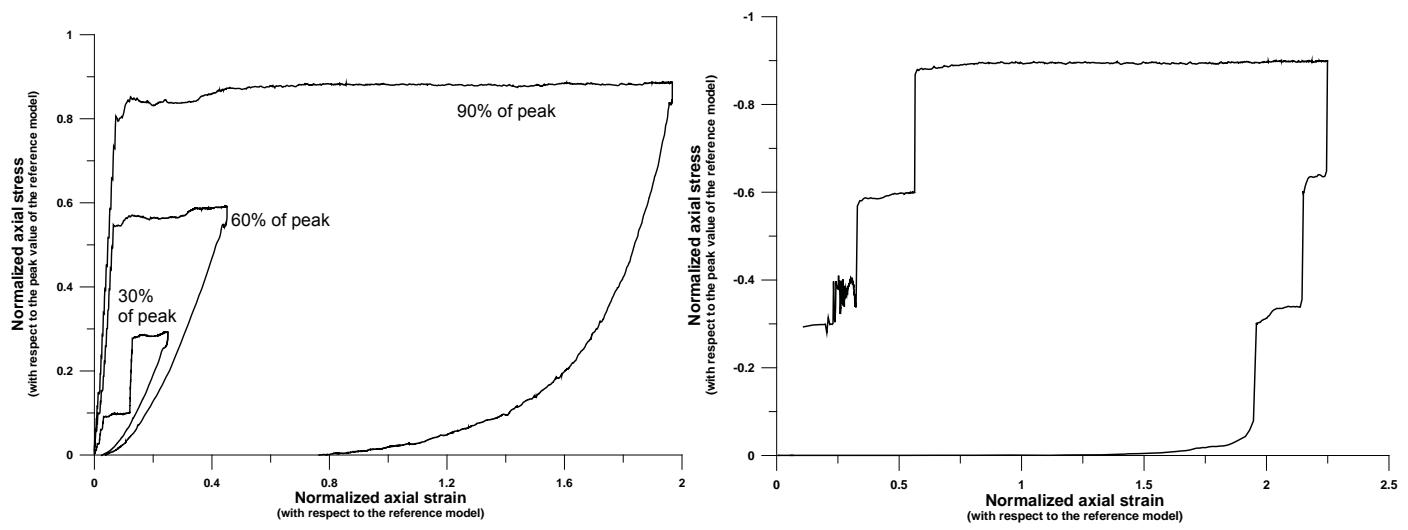


te Kamp & Konietzky 2002

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## Compaction under constant load levels (note: irreversible plastic deformations)



te Kamp & Konietzky 2002

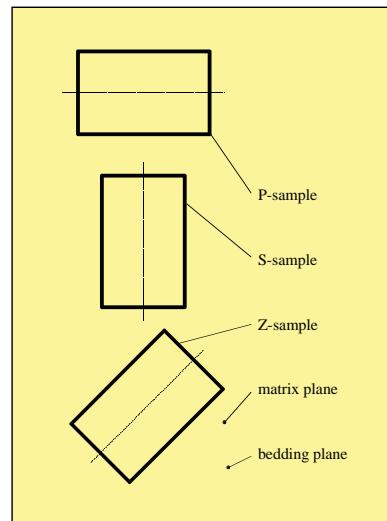
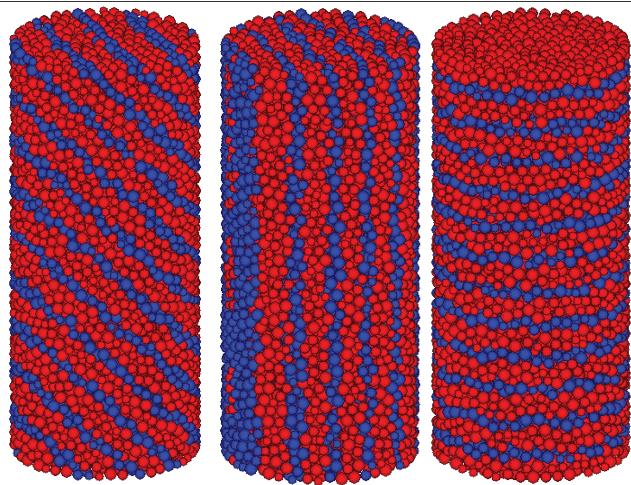
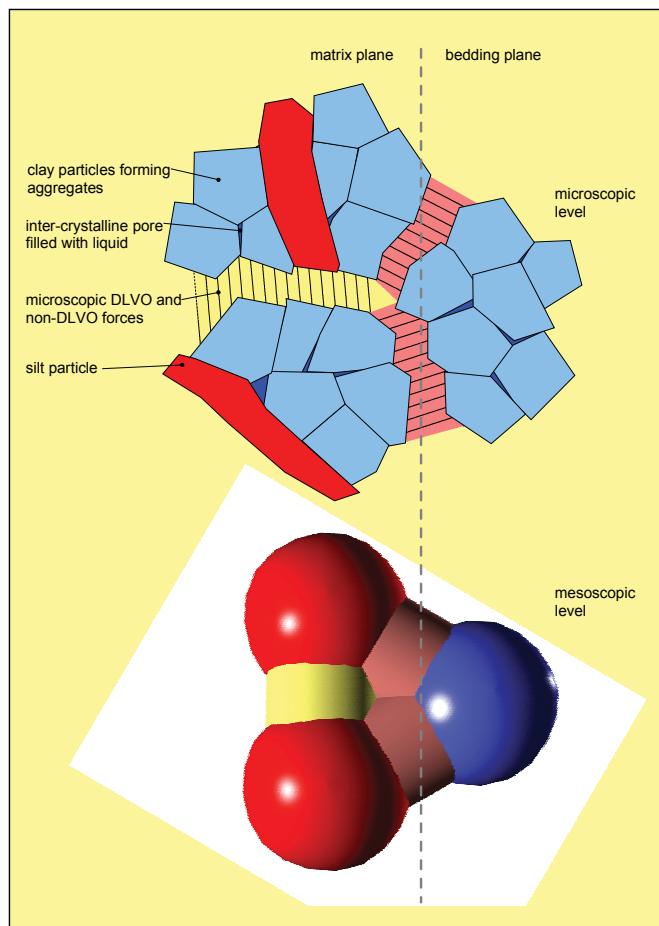
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„Physical“ concept  
at the meso-scale

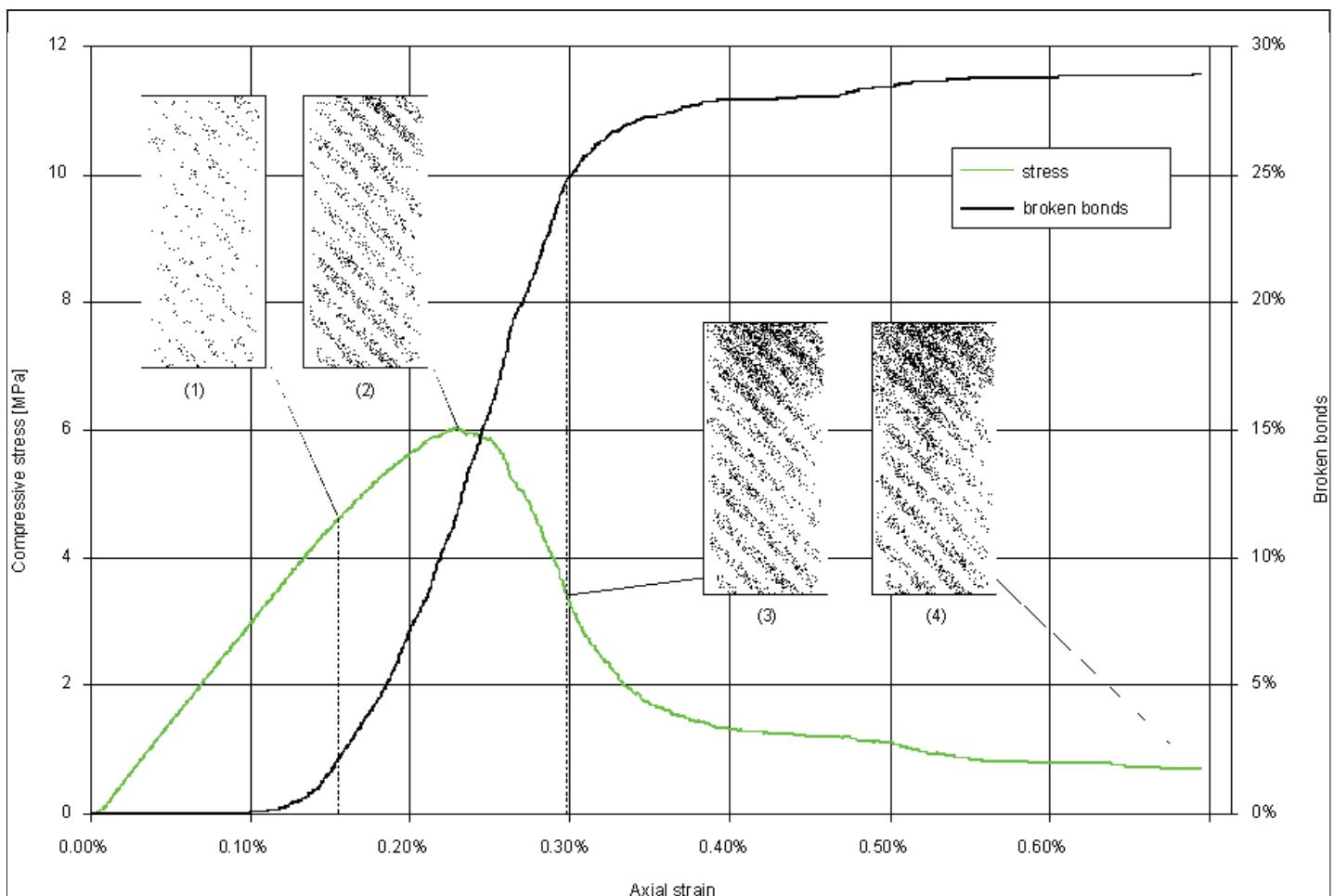


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## Anisotropic model for Opalinus Clay



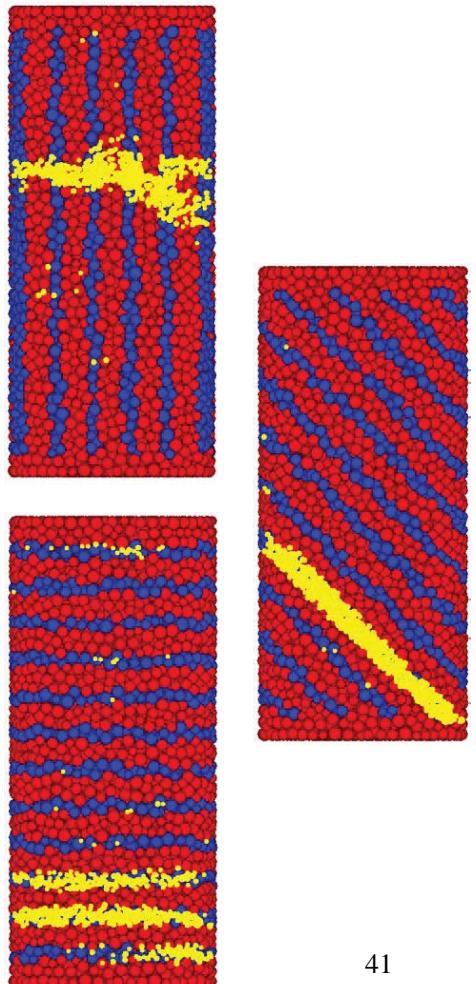
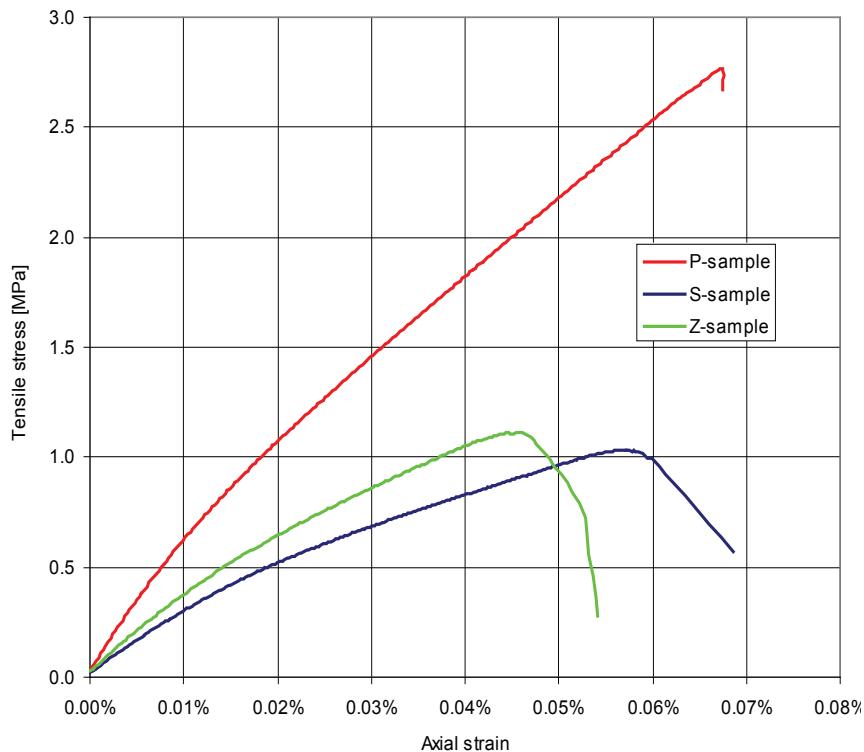
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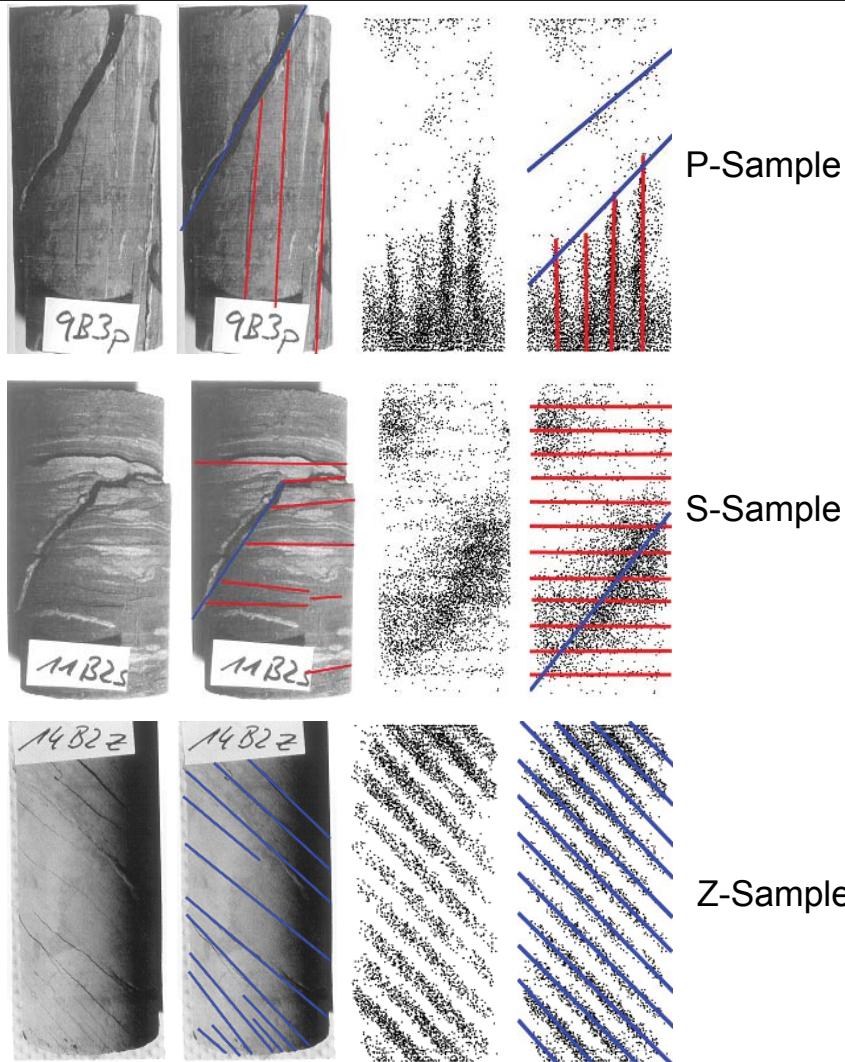
Stress – strain behaviour and fracture pattern: uniaxial compression test (S-Sample)

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## Uniaxial tensile testing: stress-strain curves and fracture pattern

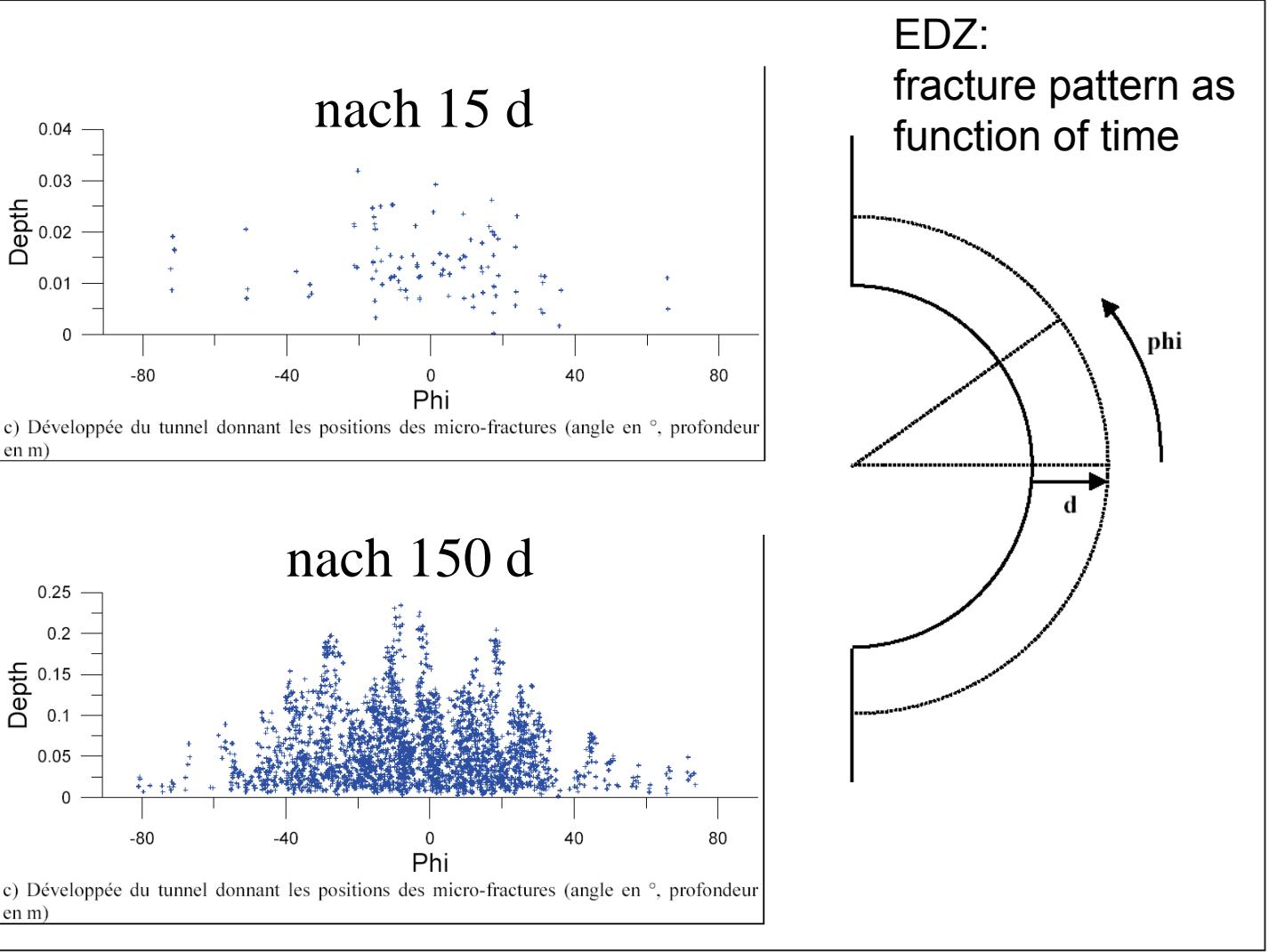


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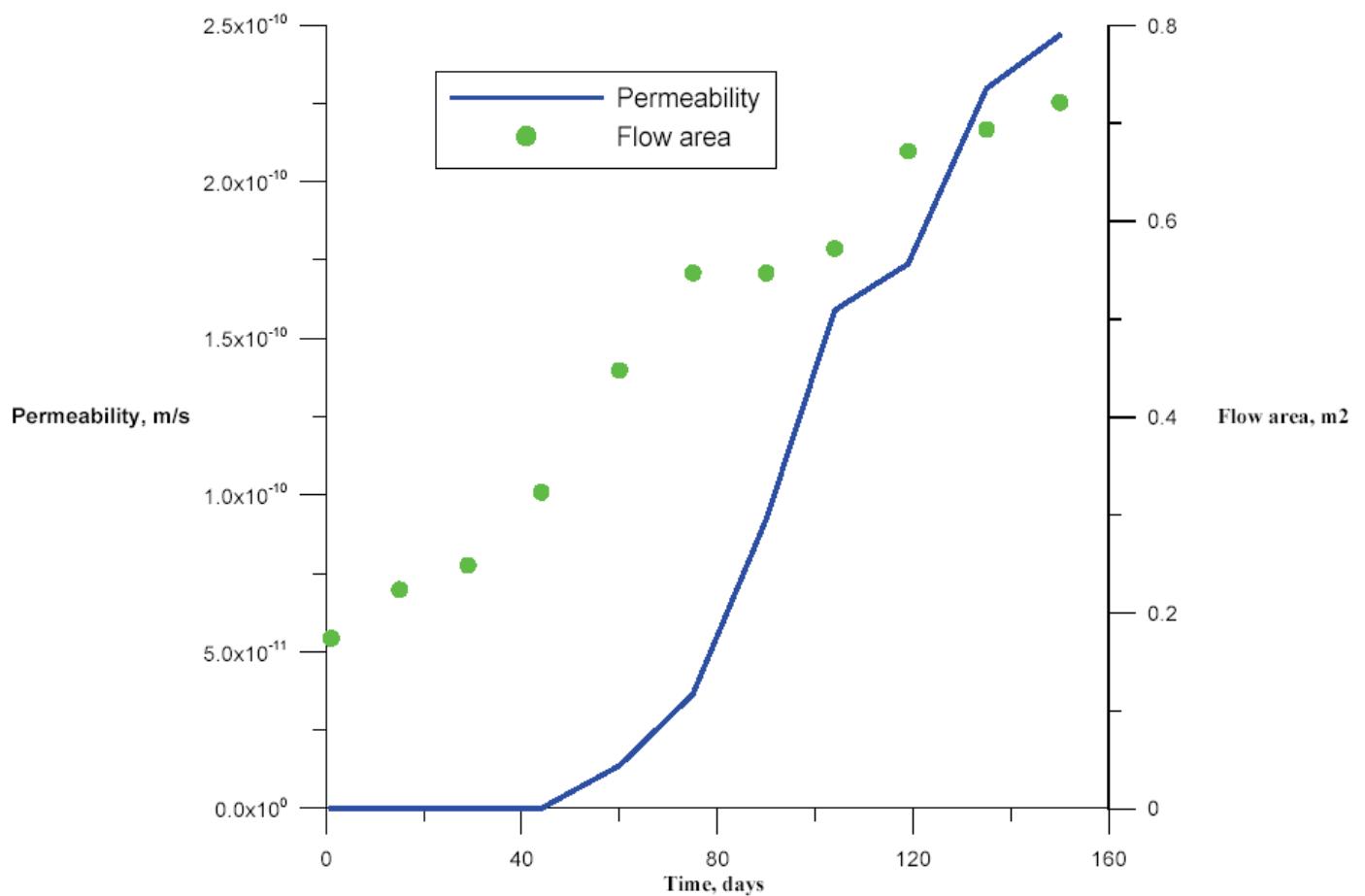


Uniaxial  
compression:  
fracture pattern  
lab vs. model

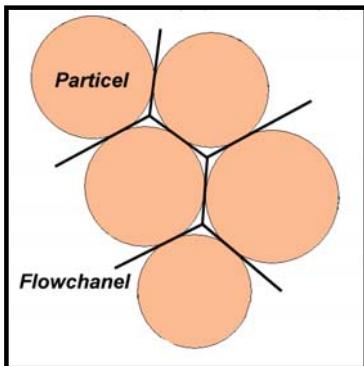
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### Permeability and flow area development in EDZ vs. time



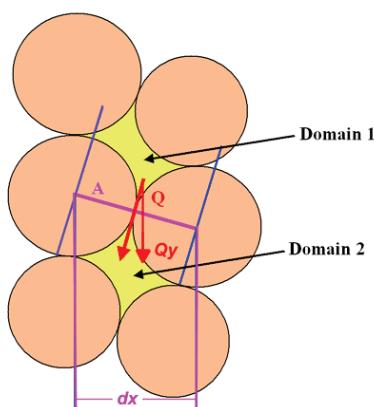
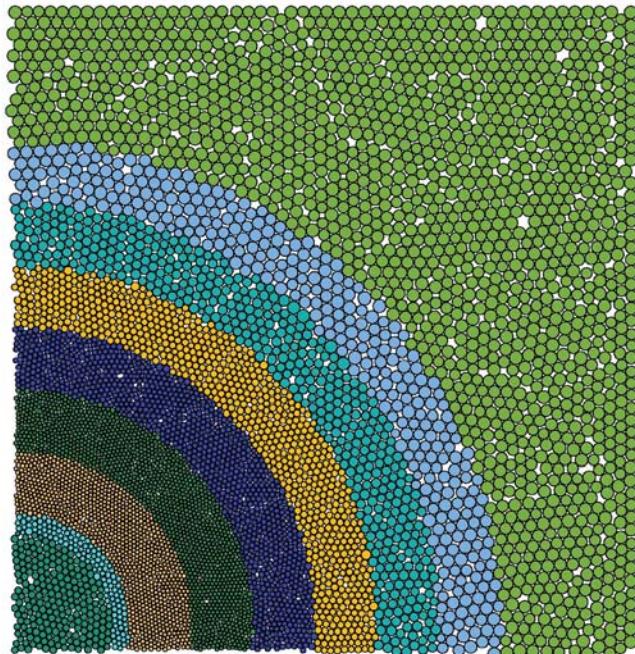
# EDZ-study: Mt. Terri, tunnel radius = 1.8 m



$$\Delta P = -K \frac{\Delta V}{V}$$

$$\dot{Q} = K a^3 \frac{\Delta P}{\Delta X}$$

$$a = \frac{a_0 F_0}{F + F_0}$$



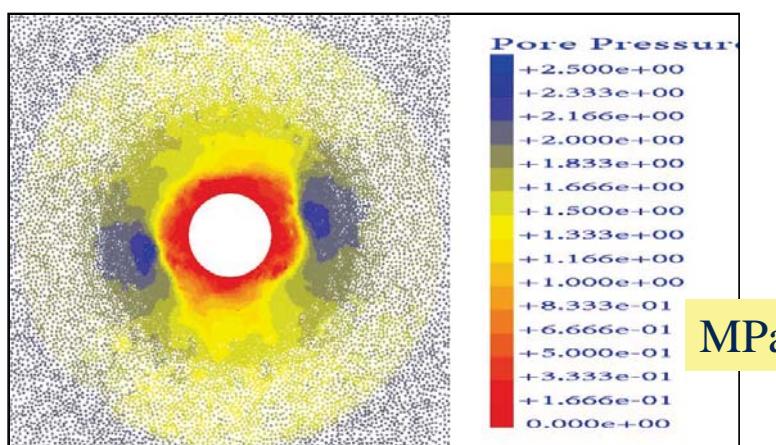
Numerical model set-up and  
Illustration of HM-coupling scheme

te Kamp, Konietzky & Blümling 1999  
Konietzky, te Kamp & Blümling 2001

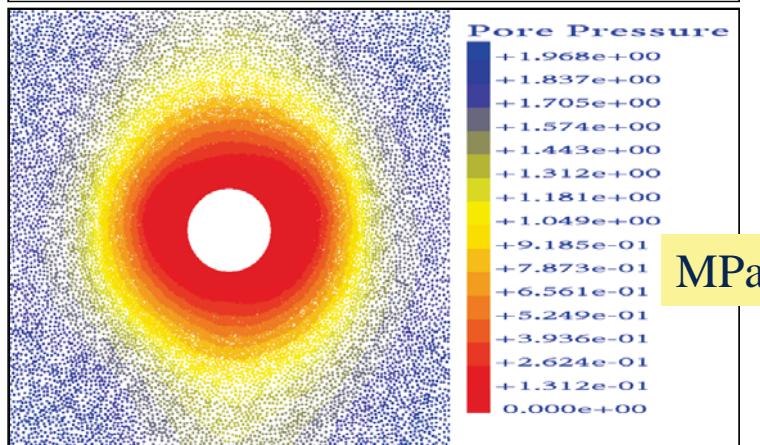
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$P_{p,ini}=2 \text{ MPa}$

1 day



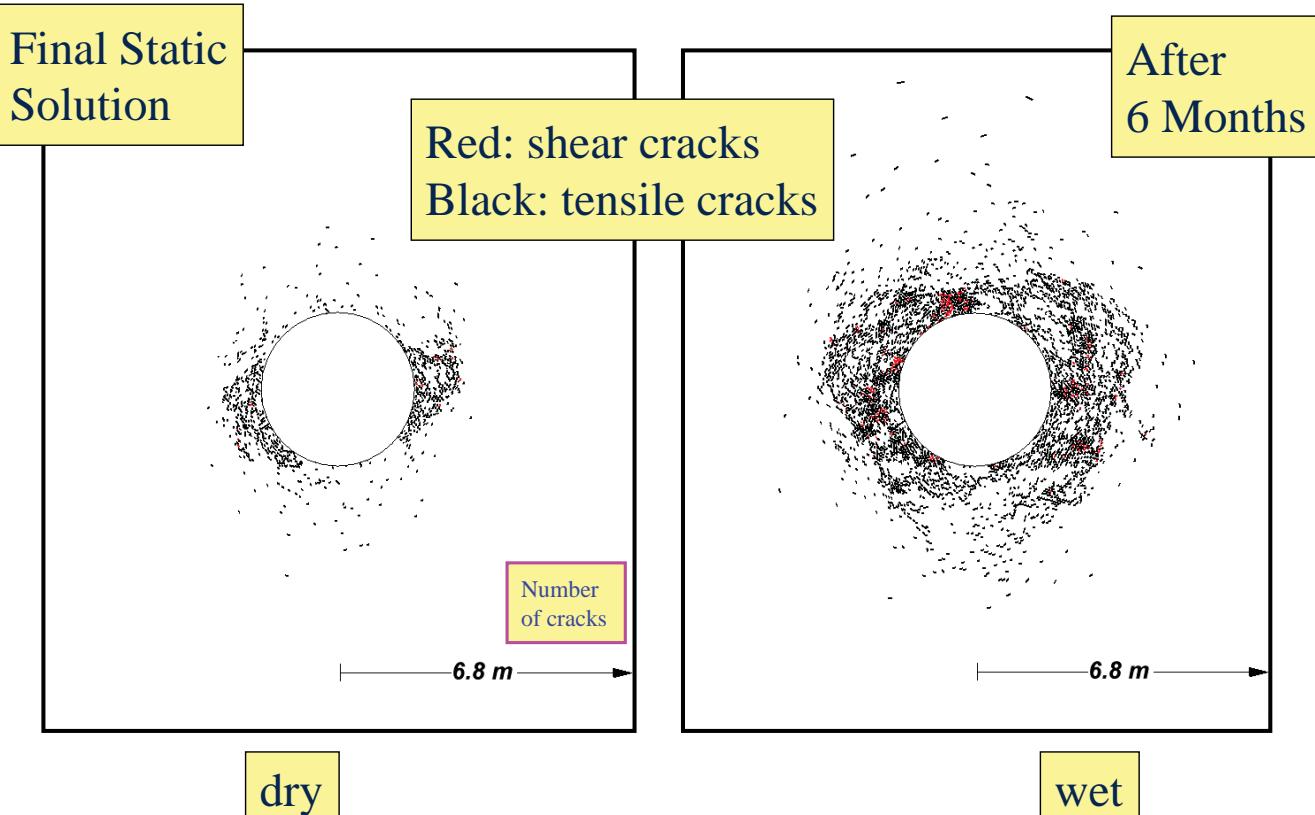
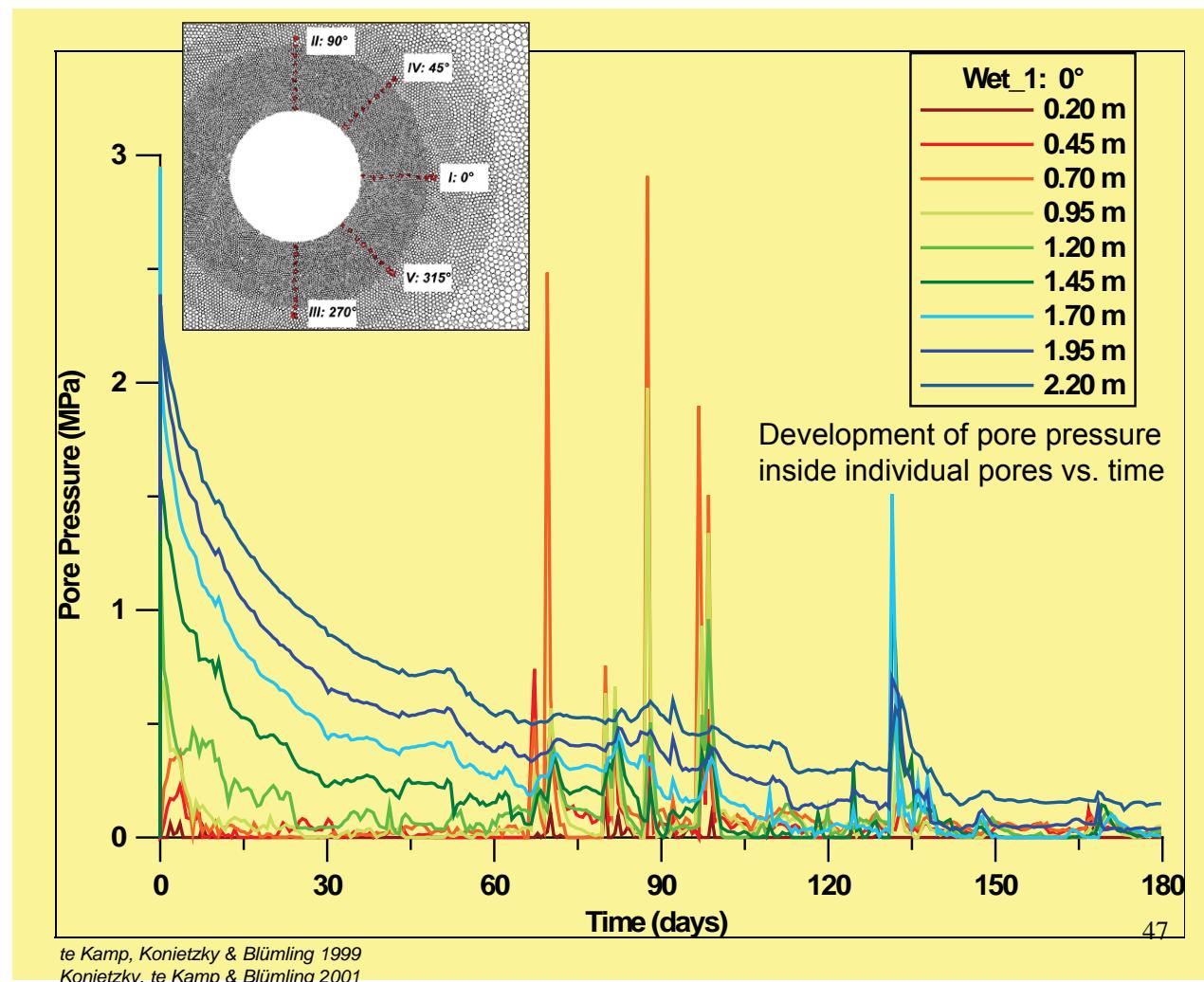
1 month



Pore pressure distribution around opening

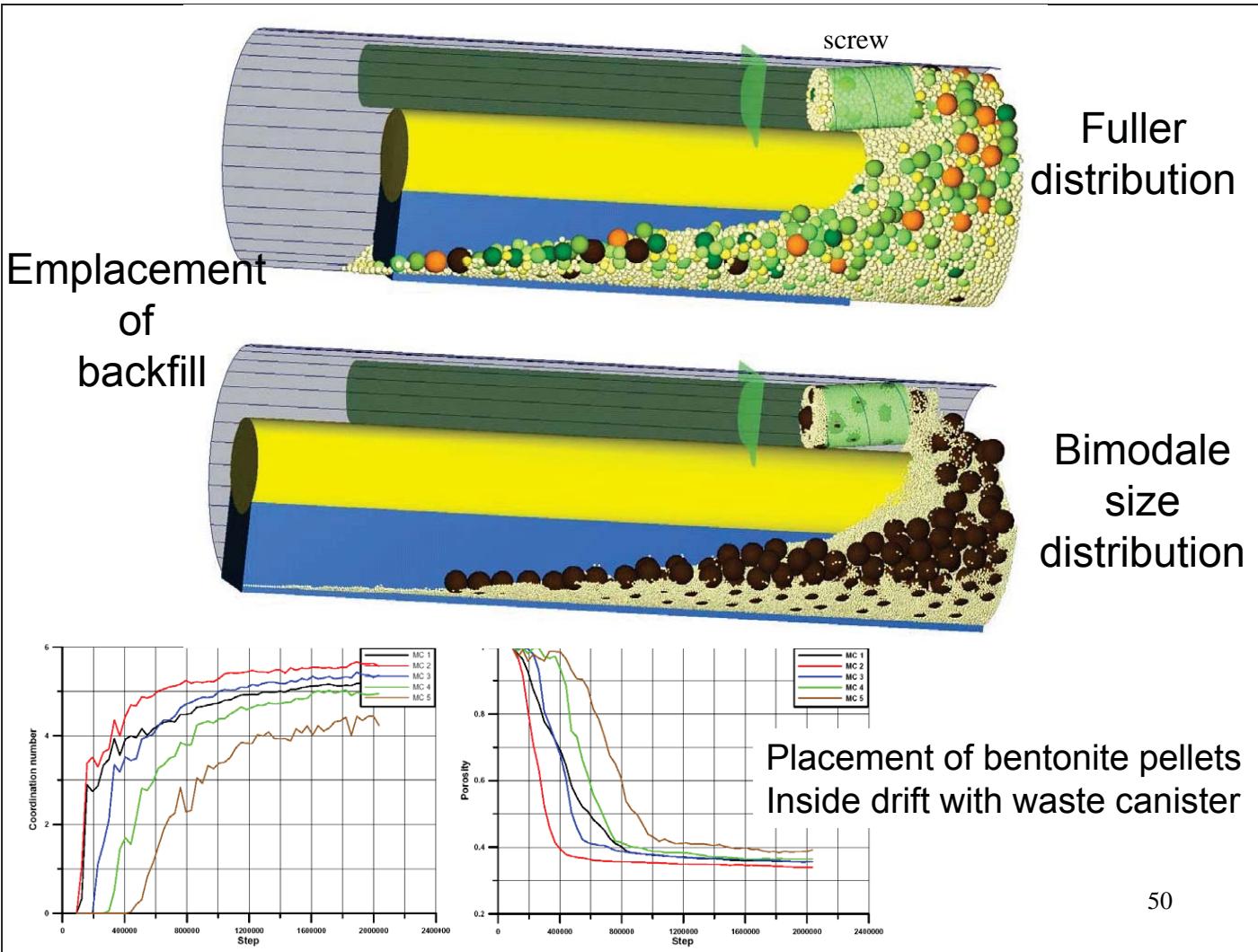
te Kamp, Konietzky & Blümling 1999  
Konietzky, te Kamp & Blümling 2001

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Comparison: damage state under dry and wet conditions

# Simulation potential at the meso/macro-scale based on DEM technique



Verständnis mikromech. Prozesse = Voraussetzung für fundierte Prognose

Knowledge micromech. Processes = Prerequisite for reliable Prediction

Correct micro- and meso-mechanical simulation demands the explicit consideration of:

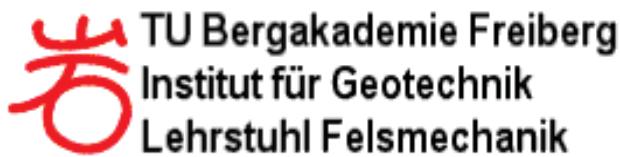
- Grain shapes
- Grain size distribution
- Initial damage
- Intragranular and intergranular fracturing
- Porosity (shape, size, distribution)
- Mineral components / phases
- Critical and subcritical crack growth
- Simulation of granular flow and compaction

Korrekte mikro- und mesomechanische Simulationen erfordern die explizite Berücksichtigung von:

- Kornform
- Korngrößenverteilung
- Initiale Schädigung
- Intragranulare und intergranul. Bruchprozesse
- Porosität (Form, Größe, Verteilung)
- Mineralbestand
- Kritisches und subkritisches Risswachstum
- Simulation of Partikelströmen und Kompaktion

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**Thanks for your kind attention**



Following co-workers have contributed to the presented results:

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