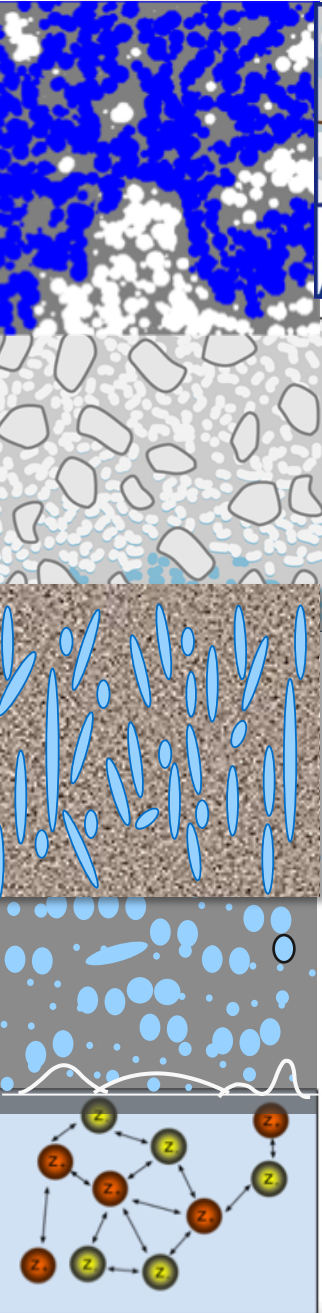


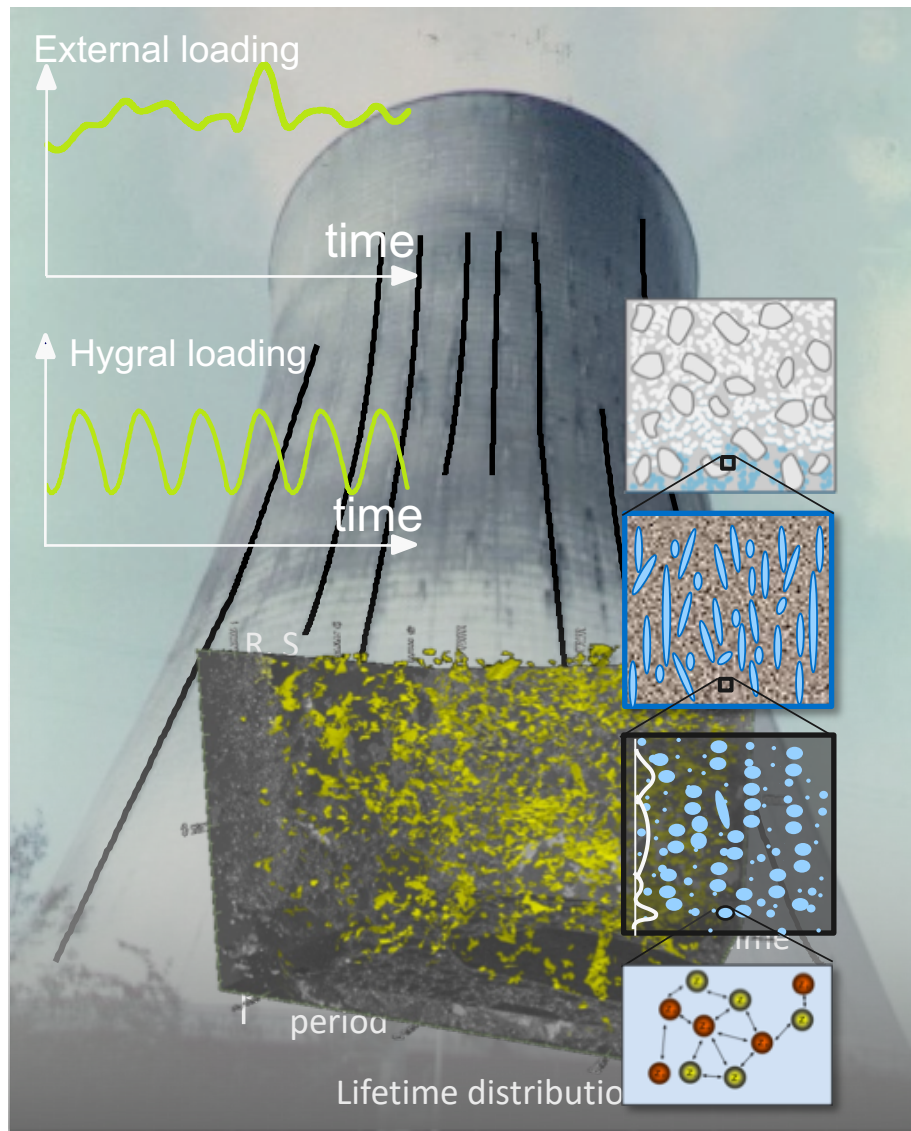


Scale traversing models for durability oriented computational analyses of concrete and concrete structures

Günther Meschke

J. J. Timothy, T. Iskhakov, M. Hofmann

Institute for Structural Mechanics
Ruhr University Bochum

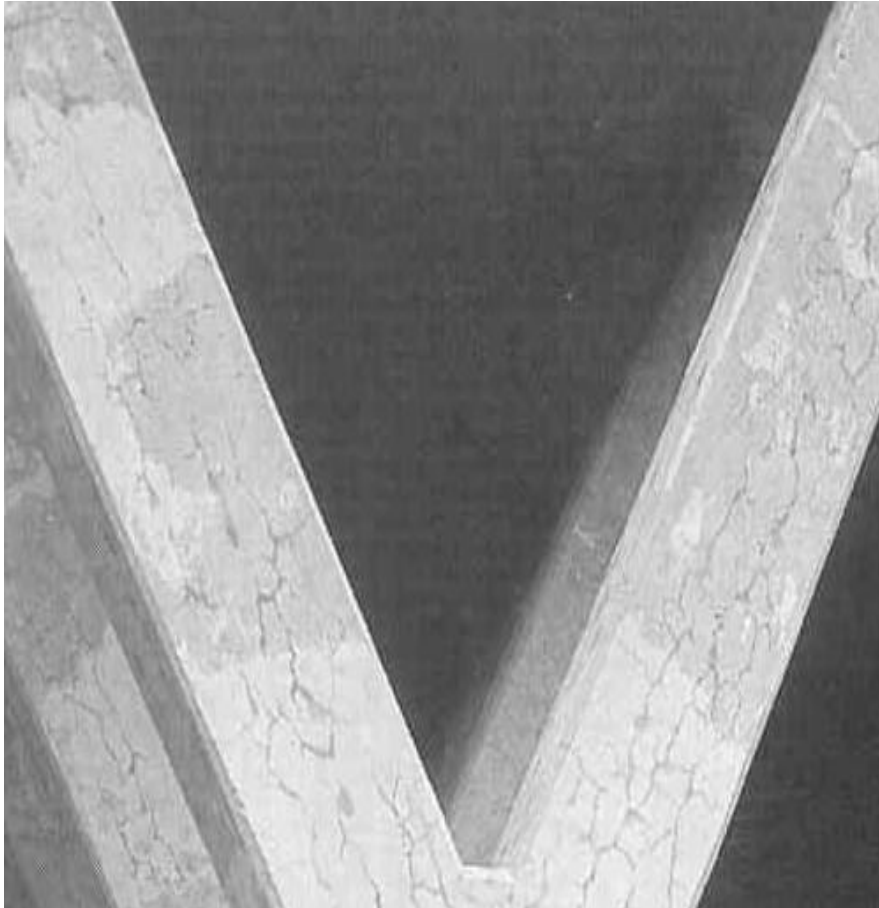


Long-term structural degradation:

- Coupled processes
- load carrying capacity (ULS) , serviceability of structures affected

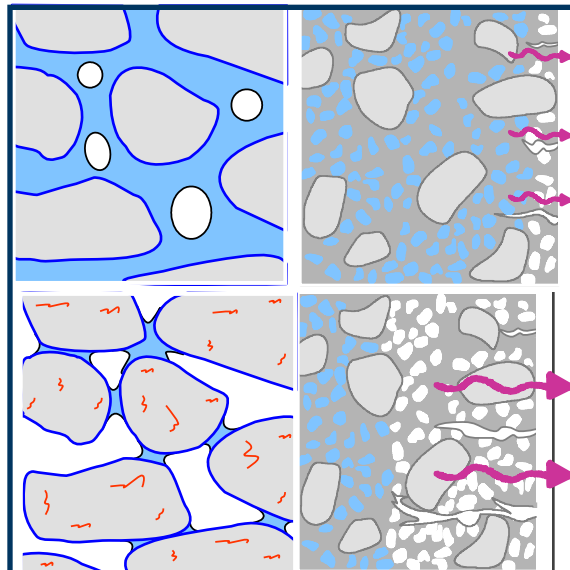
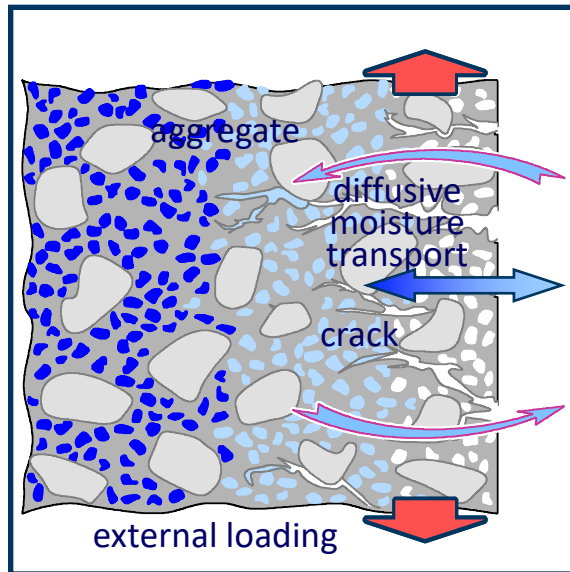
Durability analysis:

- multiphase & multifield models
- Phenomenological vs. multiscale modeling
- Multiphysics models: macroscopic stiffness, diffusivity and permeability depending on microstructure and state of damage
- Example: Moisture transport in pre-damaged concrete road pavements
- Alkali-Silica reaction: phenomenological vs. multiscale model

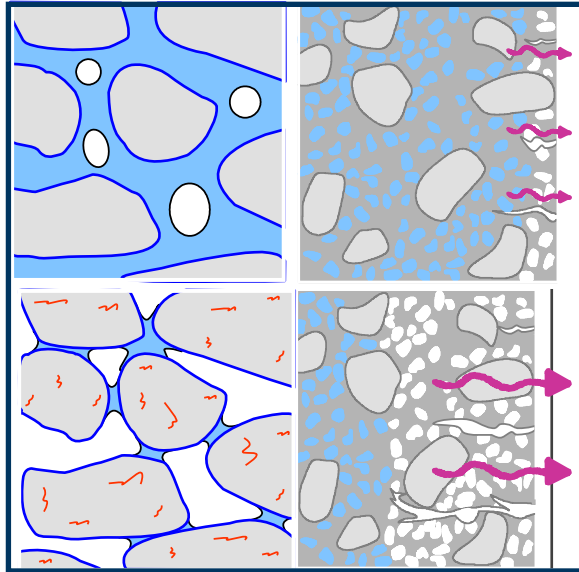


STARK & WICHT 2001

Germany: $\sim 8\%$ of Highways affected



- Diffusive moisture transport
- Capillary stresses increase with drying
- Shrinkage deformations
- Cracking due to restrained shrinkage deformations
- Cracks promote moisture transport
- Moisture changes microprestress in gelpores
- Drying promotes creep deformations (Pickett-Effect)
- Three-field (u, p_g, p_l) and two-field formulations (u, p_c) in the framework of the Biot-Coussy Theory of porous media
- Hygro-mechanical couplings considered – damage - drying shrinkage, drying creep



Porosity:

$$\phi = \phi_l + \phi_g,$$

Balance of momentum:

$$\text{div } \boldsymbol{\sigma} + \mathbf{b} = 0$$

Balance of mass of pore fluid:

$$\text{div } q_l + \dot{m} = 0$$

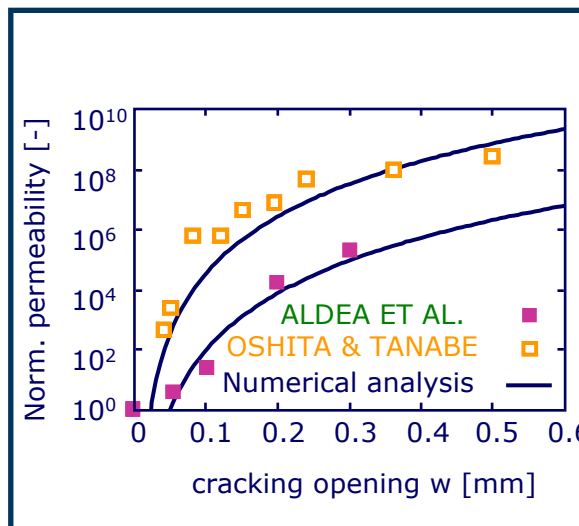
Moisture transport:

$$q_l = \frac{\rho_l}{\eta_l} k_r(S_l) [k_\phi(\phi) \mathbf{k}_0 + \mathbf{k}_d(d)]$$

Constitutive relations:

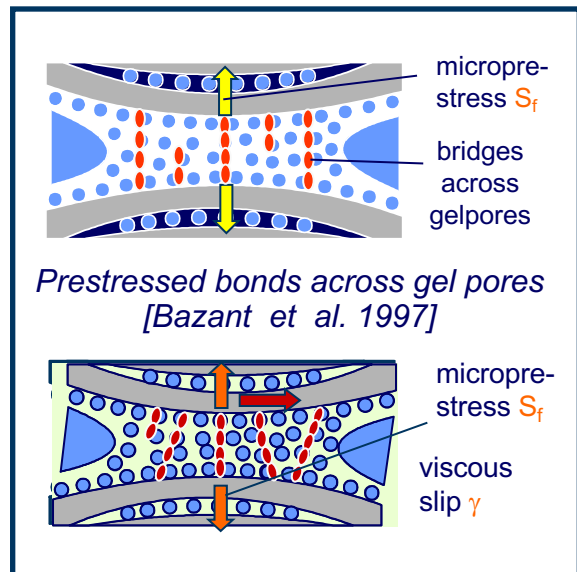
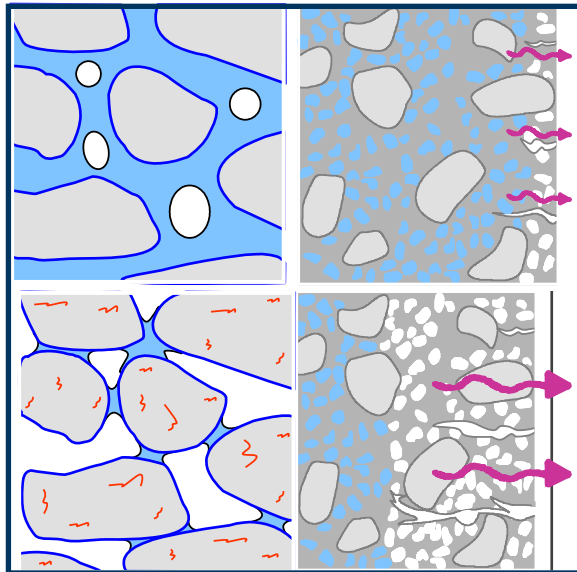
$$\boldsymbol{\sigma} = \nabla_{\boldsymbol{\varepsilon}^e} \psi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^p, \boldsymbol{\varepsilon}^f, m_l, d, \gamma)$$

$$p_c = \nabla_{\phi_l^e} \psi(\boldsymbol{\varepsilon}^e, m_l, \phi_l^p, d, \gamma)$$



Coussy 2005, GM & Grasberger, S. (2003) ASCE Engineering Mechanics

Phenomenological model: Drying shrinkage, damage and creep



Porosity:

$$\phi = \phi_l + \phi_g,$$

Balance of momentum:

$$\text{div } \boldsymbol{\sigma} + \mathbf{b} = 0$$

Balance of mass of pore fluid:

$$\text{div } q_l + \dot{m} = 0$$

Moisture transport:

$$q_l = \frac{\rho_l}{\eta_l} k_r(S_l) [k_\phi(\phi) \mathbf{k}_0 + \mathbf{k}_d(d)]$$

Constitutive relations:

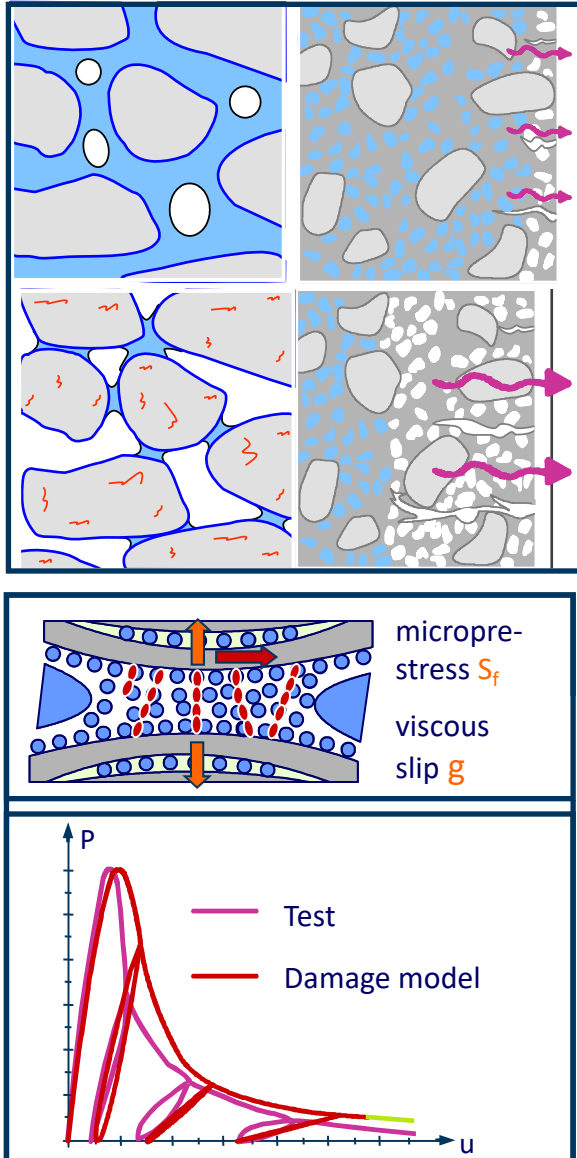
$$\boldsymbol{\sigma} = \nabla \boldsymbol{\varepsilon}^e \psi, \quad p_c = \nabla \phi_i^e \psi$$

Microprestress - driving force for long term creep

$$S_f = \nabla_{\gamma_f} \psi, \quad \dot{\varepsilon}^f = \frac{1}{\eta_f(S_f(\gamma))} \mathbf{C}^{-1} : \boldsymbol{\sigma}'(\boldsymbol{\sigma}, S_l)$$

Bazant, Hauggaard, Baweja & Ulm (1997) ASCE Engineering Mechanics
GM & Grasberger, S. (2003) ASCE Engineering Mechanics

Phenomenological model: Drying shrinkage, damage and creep



Porosity:

$$\phi = \phi_l + \phi_g,$$

Balance of momentum:

$$\text{div } \boldsymbol{\sigma} + \mathbf{b} = 0$$

Balance of mass of pore fluid:

$$\text{div } \mathbf{q}_l + \dot{m} = 0$$

Moisture transport:

$$\mathbf{q}_l = \frac{\rho_l}{\eta_l} k_r(S_l) [k_\phi(\phi) \mathbf{k}_0 + \mathbf{k}_d(d)]$$

Constitutive relations:

$$\boldsymbol{\sigma} = \nabla \boldsymbol{\varepsilon}^e \psi, \quad p_c = \nabla \phi_i^e \psi$$

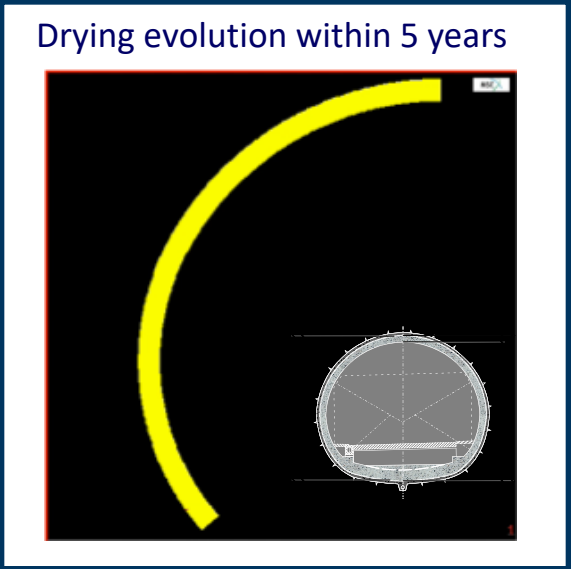
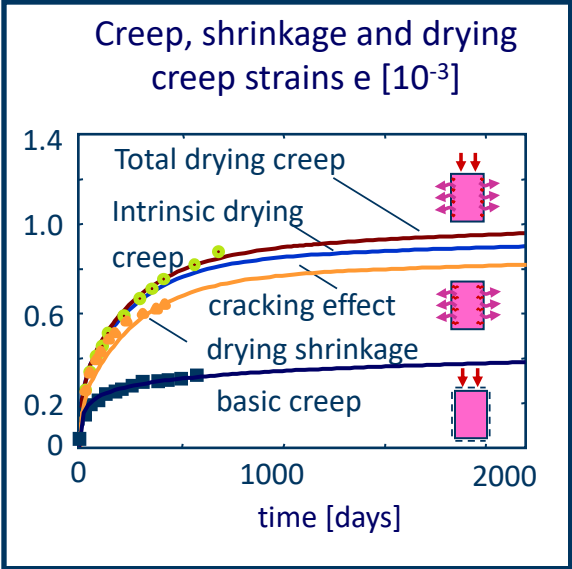
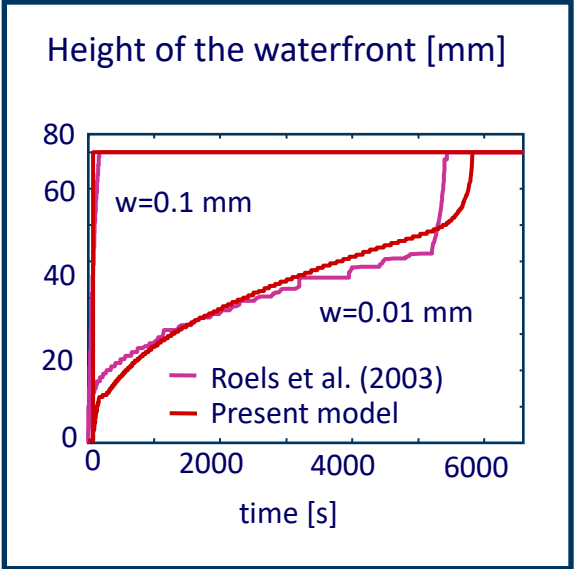
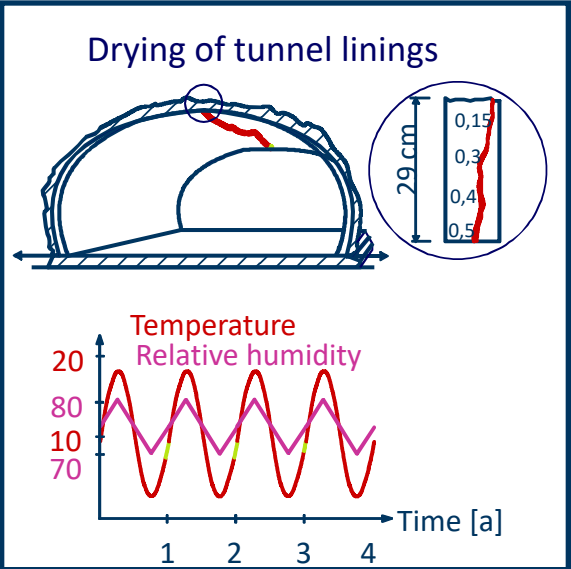
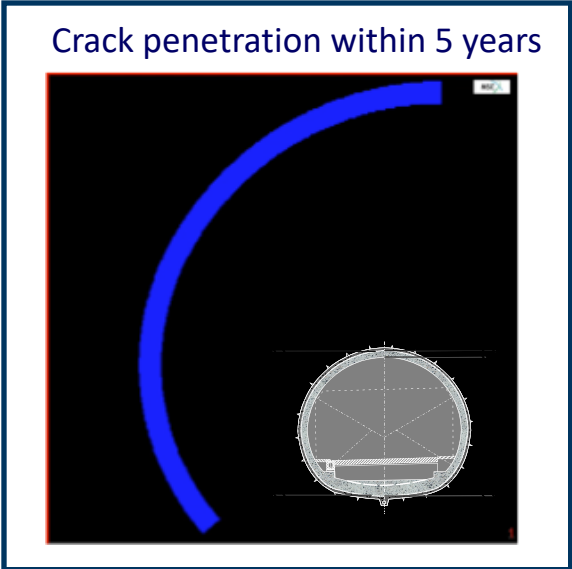
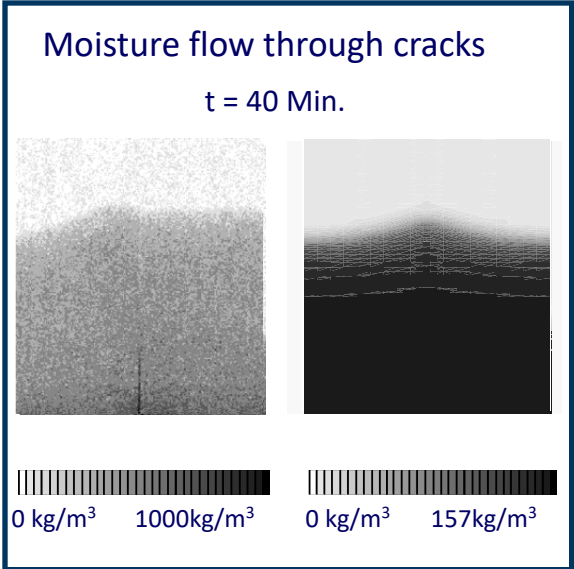
Microprestress - driving force for long term creep

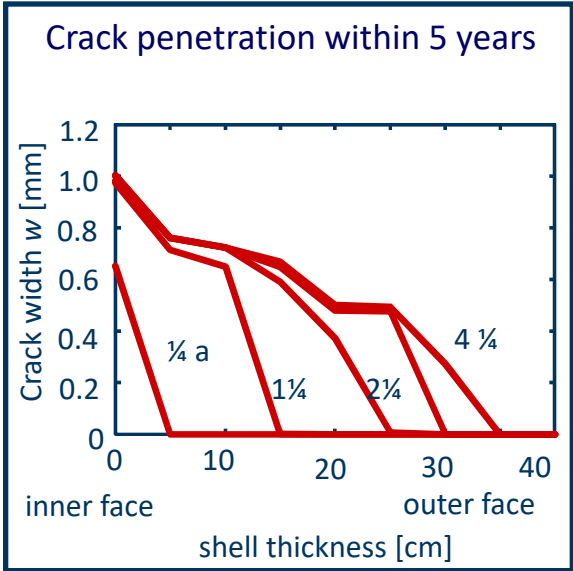
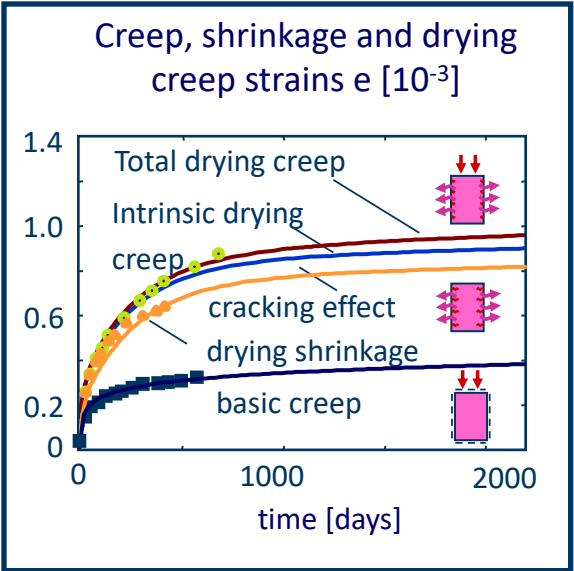
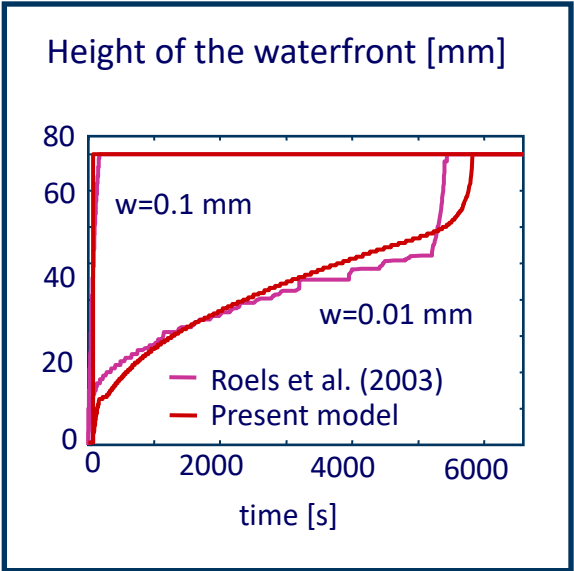
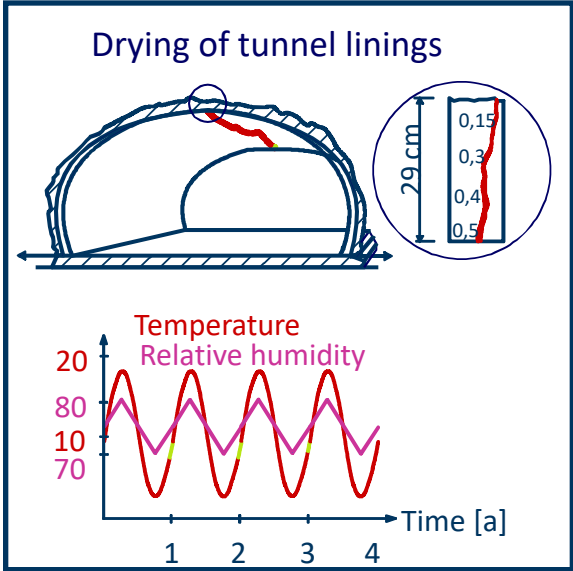
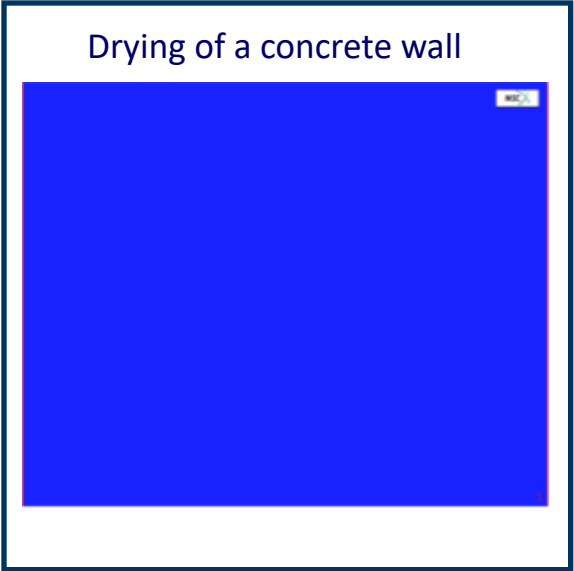
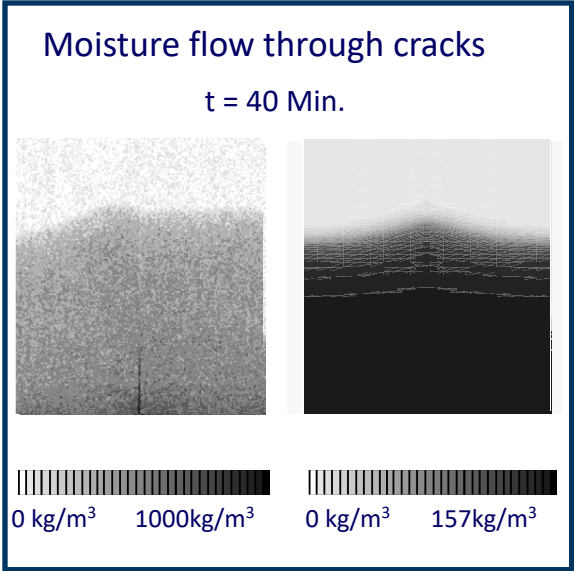
$$S_f = \nabla_{\gamma_f} \psi, \quad \dot{\boldsymbol{\varepsilon}}^f = \frac{1}{\eta_f(S_f(\gamma))} \mathbf{C}^{-1} : \boldsymbol{\sigma}'(\boldsymbol{\sigma}, S_l)$$

Multisurface plastic-damage model

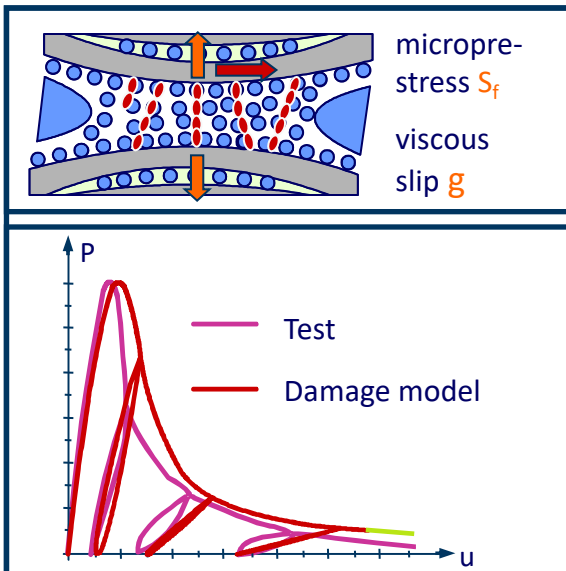
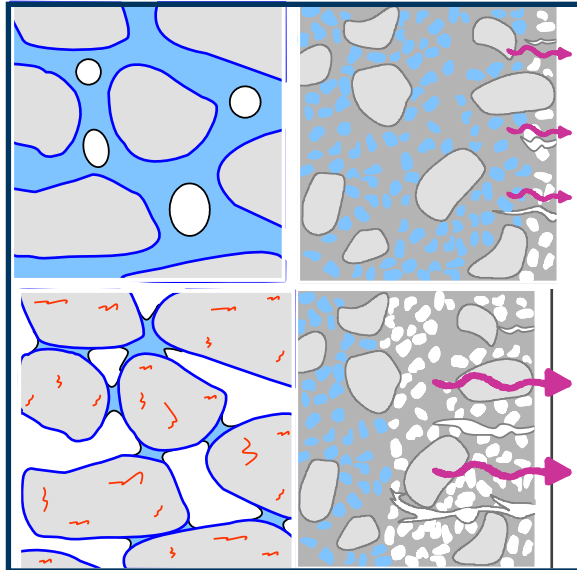
$$f_k(\boldsymbol{\sigma}, p_c, \alpha_k) \leq 0, \quad k = 1 \dots 4$$

Grasberger, S. & GM (2004), Materials and Structures,





Phenomenological model: Drying shrinkage, damage and creep



Porosity:

$$\phi = \phi_l + \phi_g,$$

Balance of momentum:

$$\text{div } \boldsymbol{\sigma} + \mathbf{b} = 0$$

Balance of mass of pore fluid:

$$\text{div } \mathbf{q}_l + \dot{m} = 0$$

Moisture transport:

$$\mathbf{q}_l = \frac{\rho_l}{\eta_l} k_r(S_l) [k_\phi(\phi) \mathbf{k}_0 + \mathbf{k}_d(d)]$$

Constitutive relations:

$$\boldsymbol{\sigma} = \nabla \boldsymbol{\varepsilon}^e \psi, \quad p_c = \nabla \phi_i^e \psi$$

Microprestress - driving force for long term creep

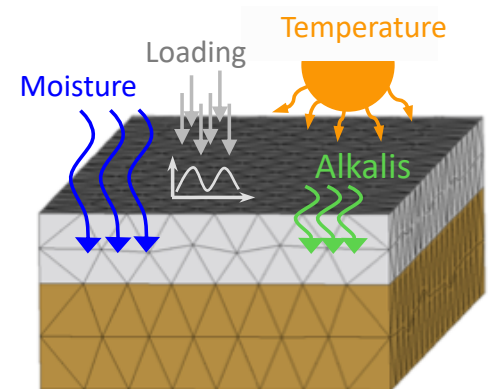
$$S_f = \nabla_{\gamma_f} \psi, \quad \dot{\boldsymbol{\varepsilon}}^f = \frac{1}{\eta_f(S_f(\gamma))} \mathbf{C}^{-1} : \boldsymbol{\sigma}'(\boldsymbol{\sigma}, S_l)$$

Multisurface plastic-damage model

$$f_k(\boldsymbol{\sigma}, p_c, \alpha_k) \leq 0, \quad k = 1 \dots 4$$

Grasberger, S. & GM (2004), Materials and Structures,

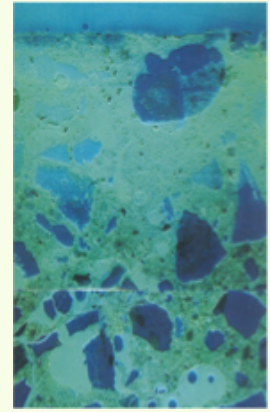
Durability of concrete infrastructure: A multiscale perspective



ASR damage in Road surfaces



ASR damage in concrete structures



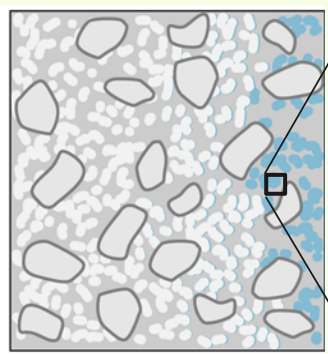
Calcium Leaching in concrete



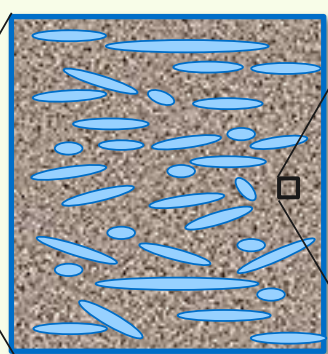
Reinforcement Corrosion

Lifetime prognosis

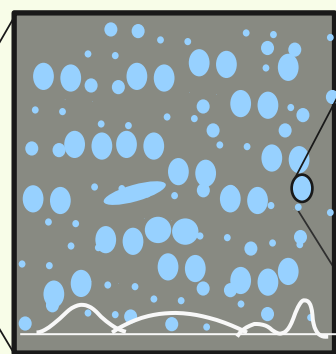
Scale-bridging Modeling



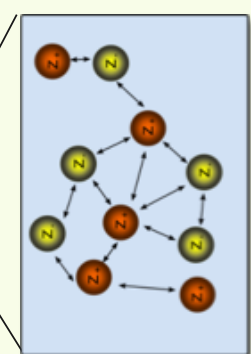
Meter



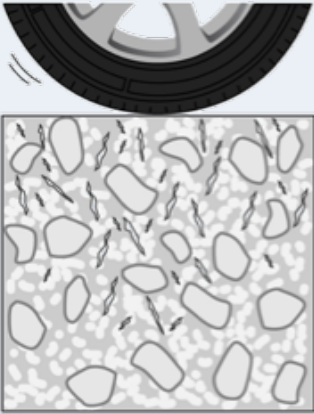
Millimeter



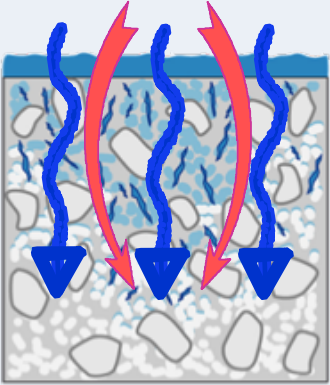
Micrometer



Nanometer



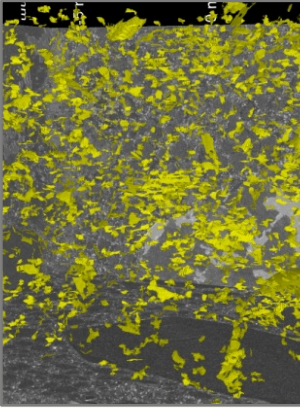
Diffuse fatigue damage in road pavements caused by traffic



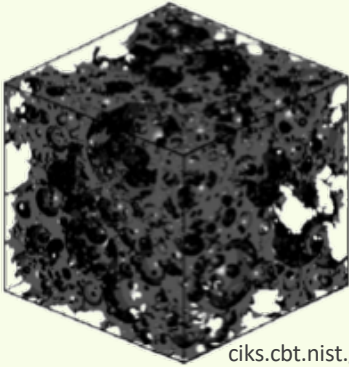
Water and Alkali transport in damaged concrete



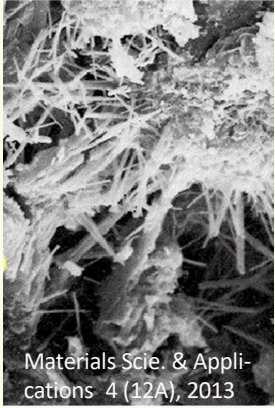
ASR damage in road surfaces



Microcracks in concrete

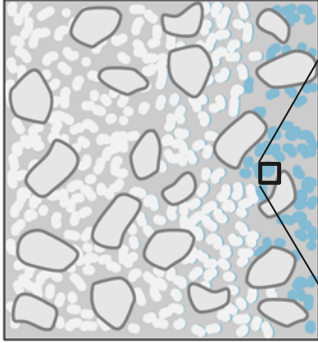


Pore space
ciks.cbt.nist.gov

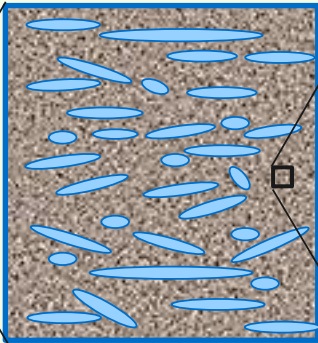


CSH phases
Materials Scie. & Applications 4 (12A), 2013

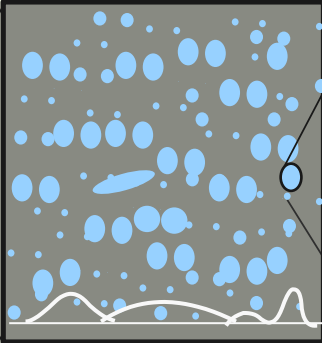
Scale-bridging Modeling of Transport processes



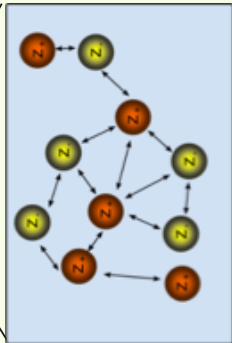
Meter



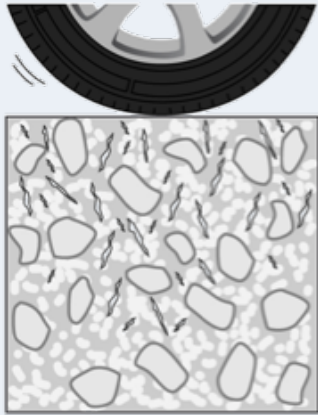
Millimeter



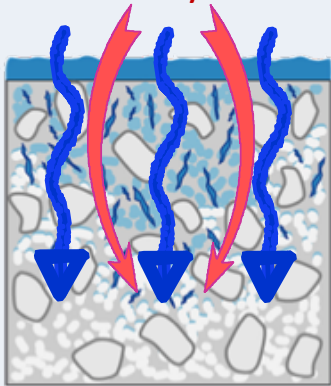
Micrometer



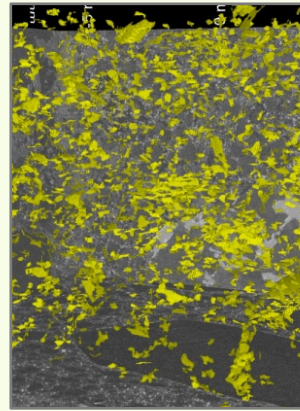
Nanometer



Diffuse fatigue damage in road pavements caused by traffic



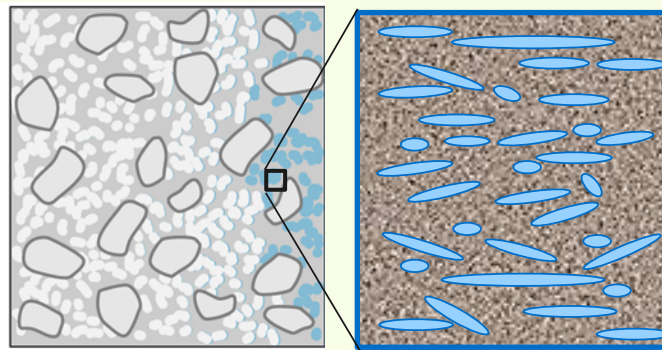
Water and Alkali transport in damaged concrete



Microcracks in concrete

Influence of microcracks on transport processes ?

Scale-bridging Modeling of Transport processes

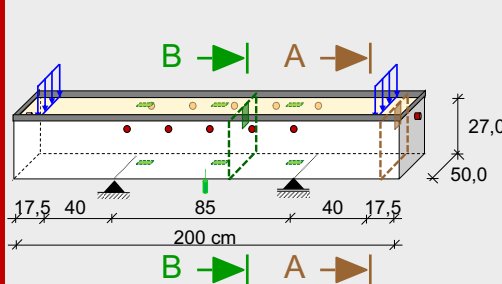


Determination of
macroscopic stiffness
diffusivity and permeability
depending on state of
damage

Influence of diffuse load-induced damage on Alkali transport in concrete



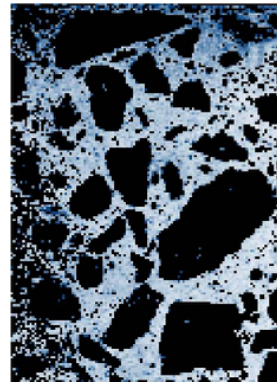
R. Przondiono et al. Beton- und Stahlbeton 2014



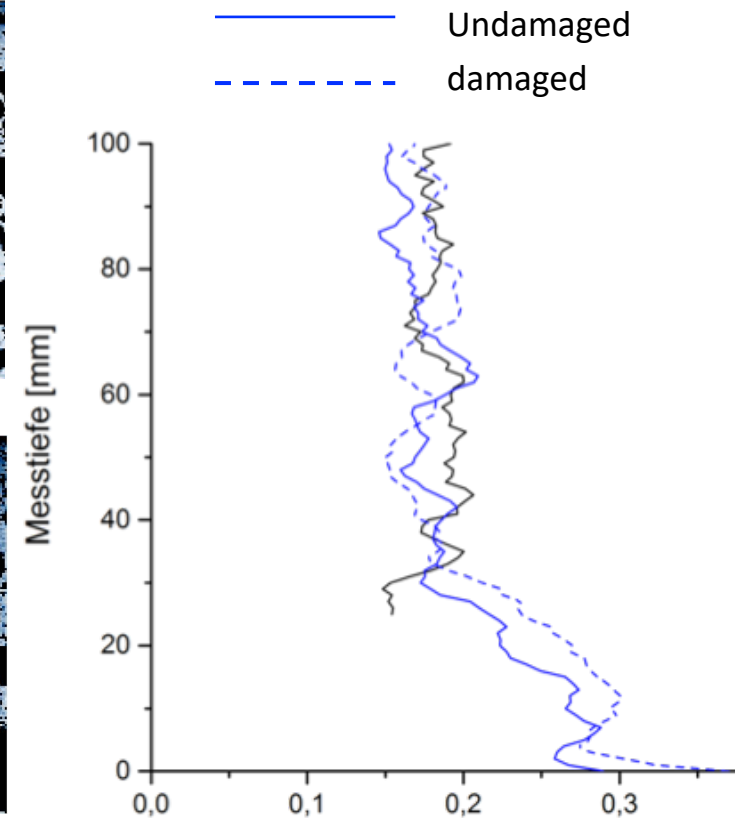
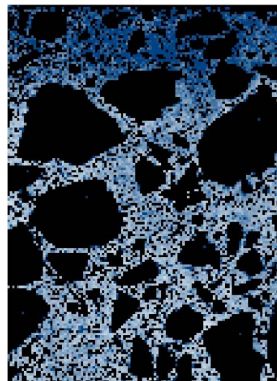
5 Mio. load cycles



Undamaged



Damaged



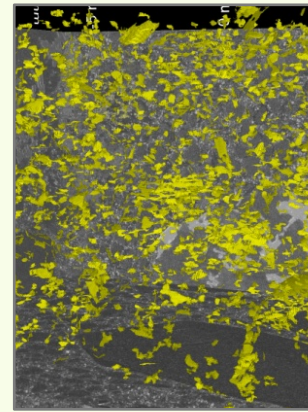
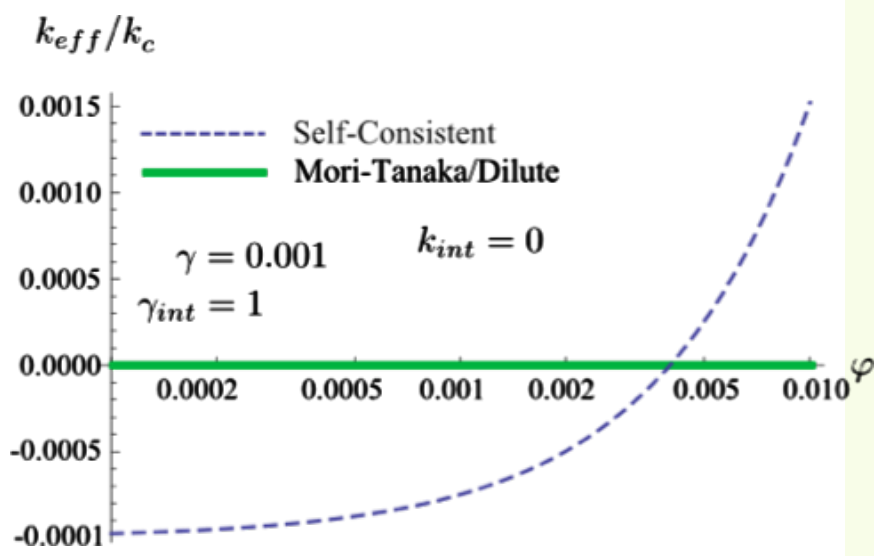
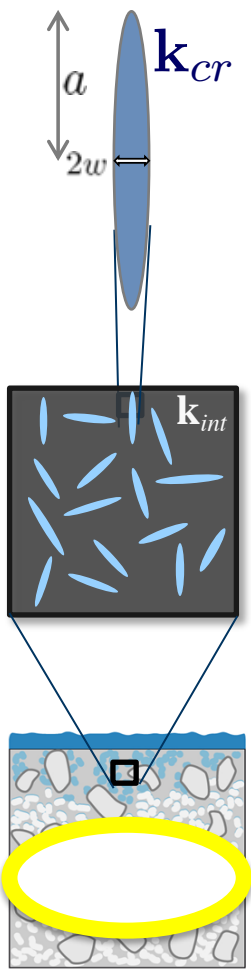
Na-profiles

F. Weise & B. Meng IBAUSIL, Weimar, 2015

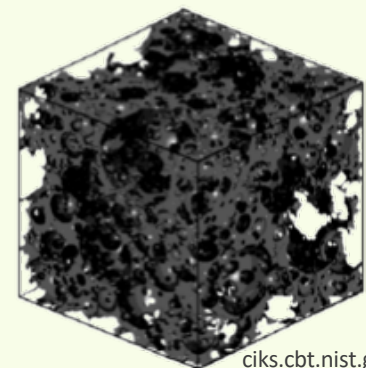
Effective Permeability of Cracked Porous Materials

Given the topology of distributed microcracks:
 What is the **effective permeability** k_{eff} ?

Does Continuum Micromechanics Homogenization methods work?



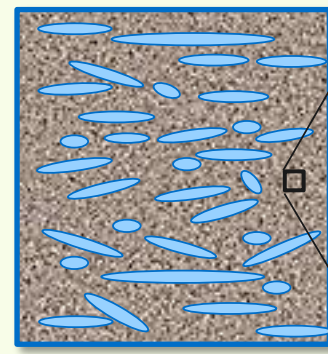
Microcracks in concrete



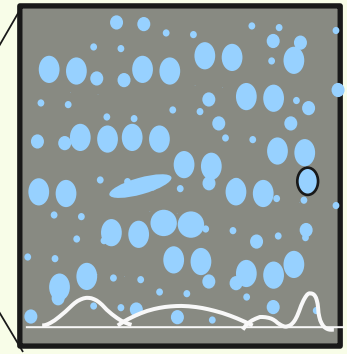
ciks.cbt.nist.gov

Pore space

Scale bridging Modeling



Millimeter



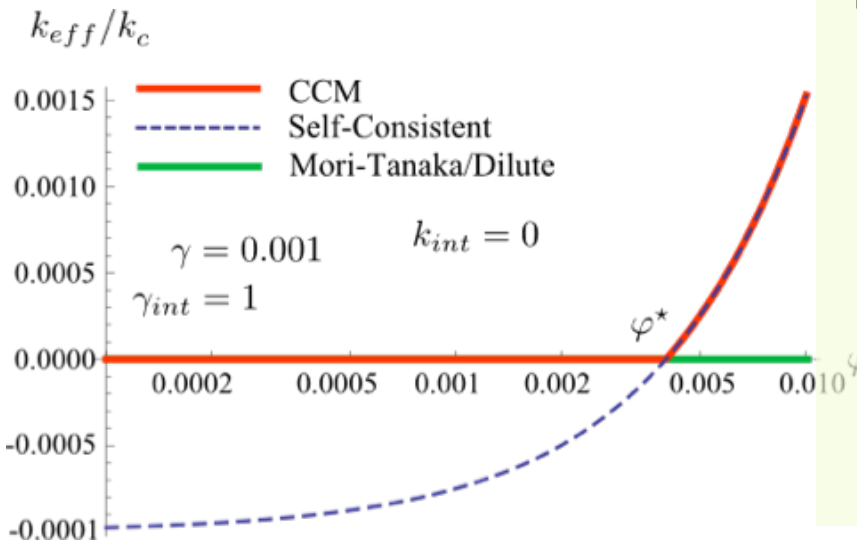
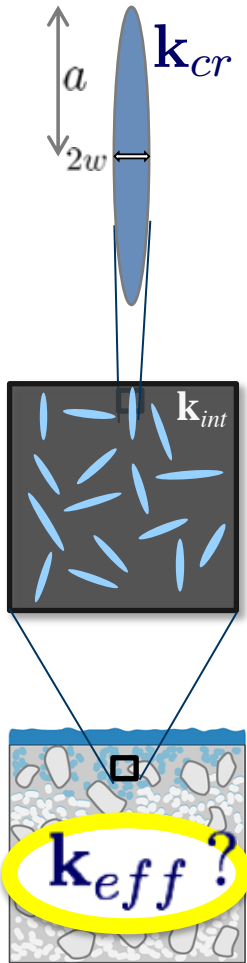
Micrometer

Effective Permeability of Cracked Porous Materials

Given the topology of distributed microcracks:

What is the **effective permeability** k_{eff} ?

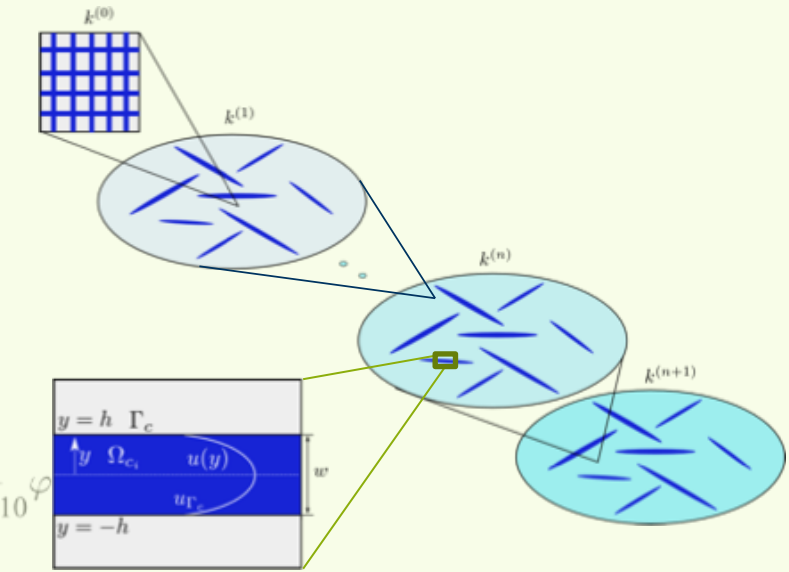
New recursive Micromechanics Model (CCM) for permeability



$$k_{eff}^{(n+1)} = \left(k_{int} (1 - \varphi) A_{int}^{(n+1)} + k_c \varphi A_c^{(n+1)} \right) \cdot B^{(n+1)}$$

$$A_c^{(n)} = K^{(n)} \cdot \left(K^{(n)} - P_c^{(n)} \right)^{-1}$$

↑ contrast ↑ shape



J. J. Timothy & GM (2016): Mechanics of Materials

Effective Permeability of Cracked Porous Materials

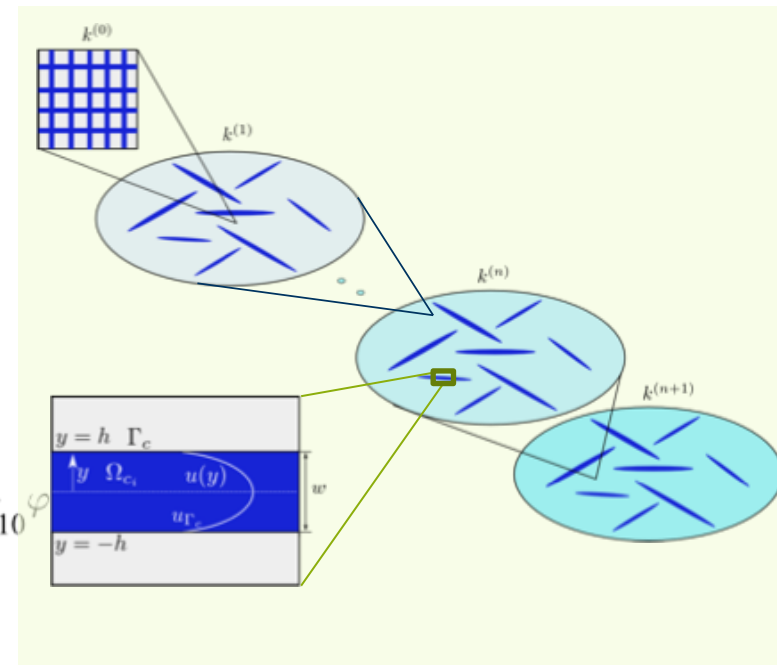
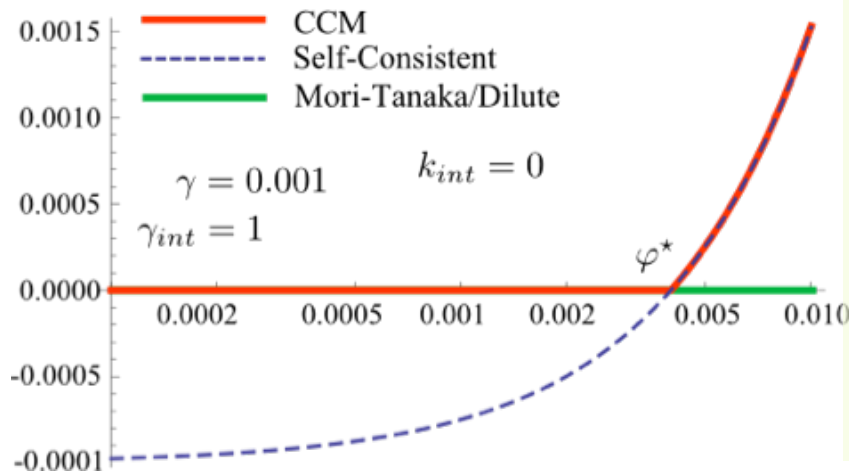
Given the topology of distributed microcracks:

What is the **effective permeability** k_{eff} ?

$$k_{eff}^{(n+1)} = \left(k_{int} (1 - \varphi) \mathbf{A}_{int}^{(n+1)} + k_c \varphi \mathbf{A}_c^{(n+1)} \right) \cdot \mathbf{B}^{(n+1)}$$

$$k_c = \frac{w^2}{12} \quad \text{not strictly valid for permeable matrix}$$

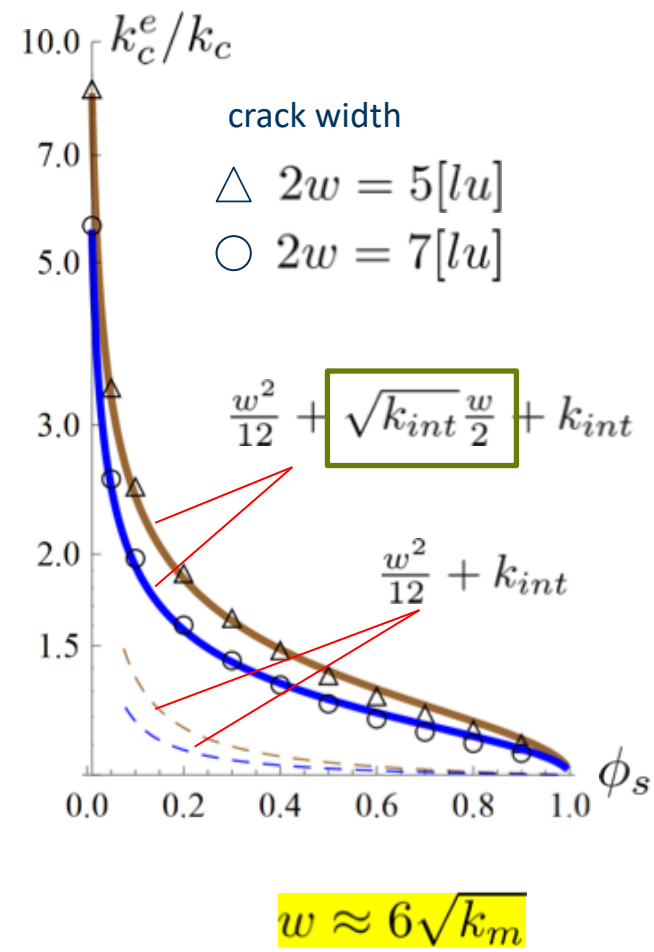
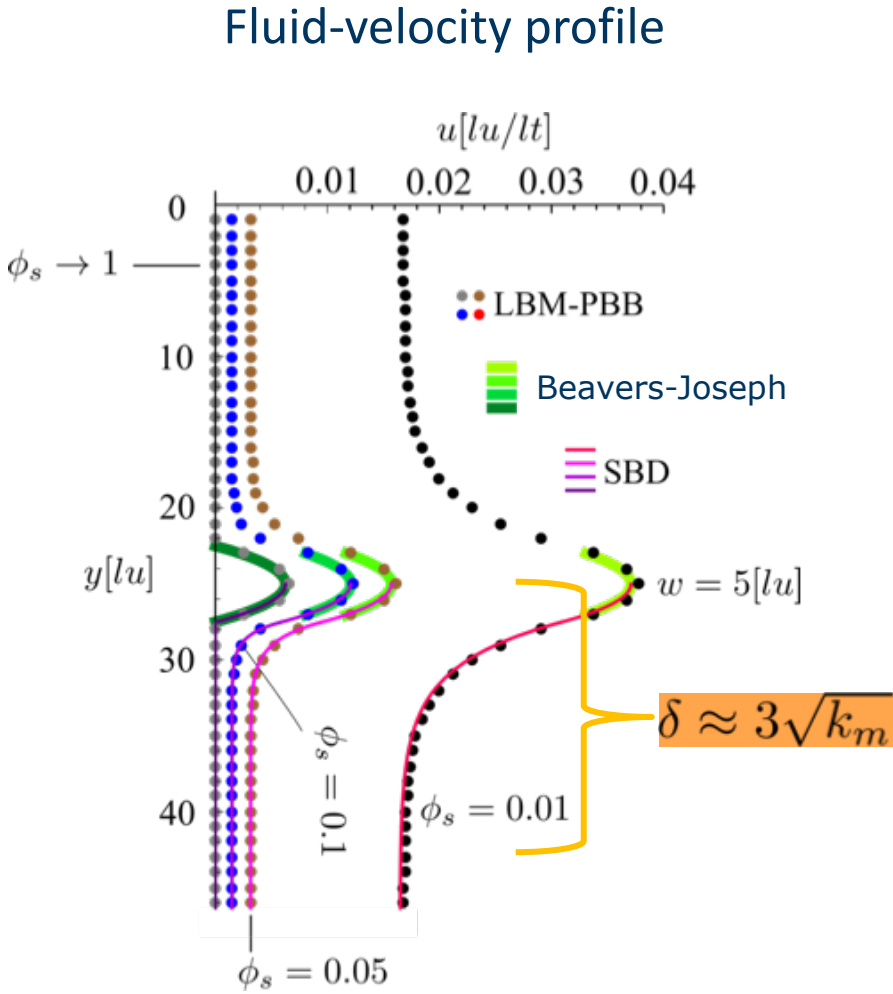
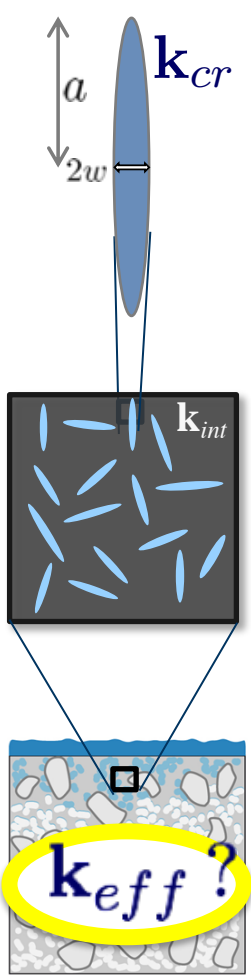
$$k_{eff}/k_c$$



New recursive Micromechanics Model (CCM) for permeability

Effective Permeability of Cracked Porous Materials

Analytical models vs. LBM-PBB simulations



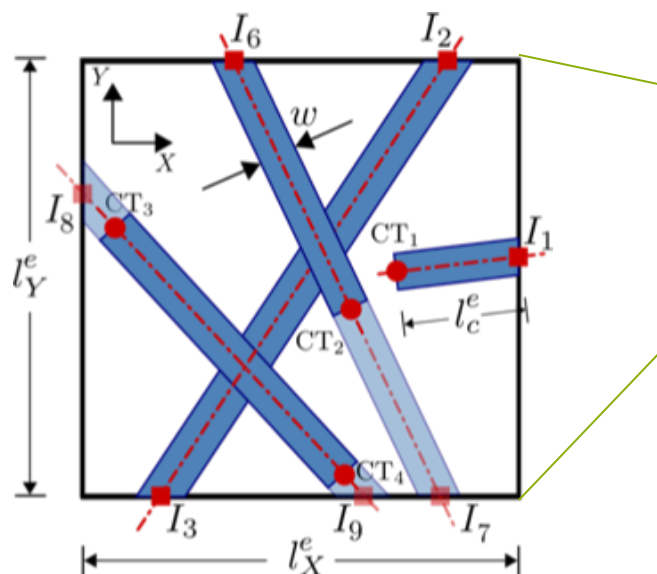
Timothy, J. J. & GM, (2017) *International Journal for Numerical and Analytical Methods in Geomechanics*.

-> cubic law not valid !

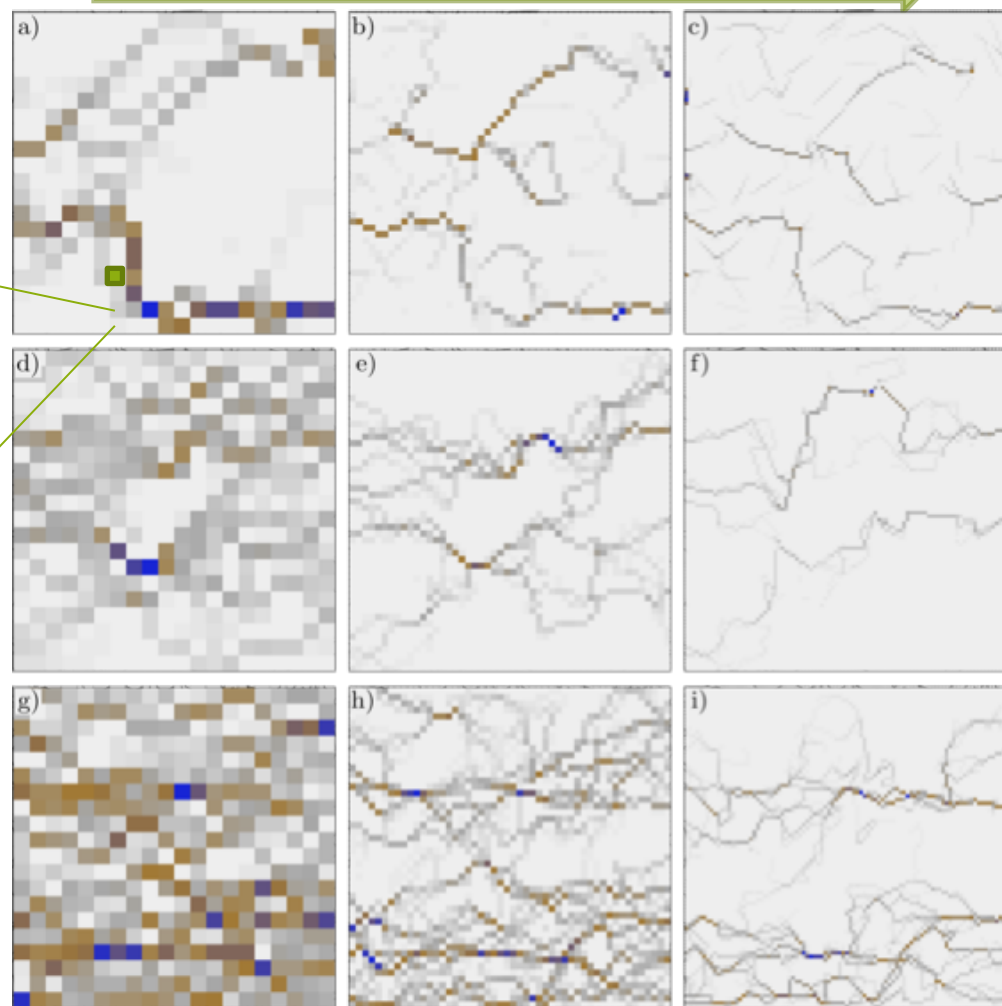
Effective Permeability of Cracked Porous Materials

Computational meso-scale analyses vs. Cascade Micromechanics Model

Effective Permeability computed for different microcrack densities and FE meshes



Resolution of numerical REV



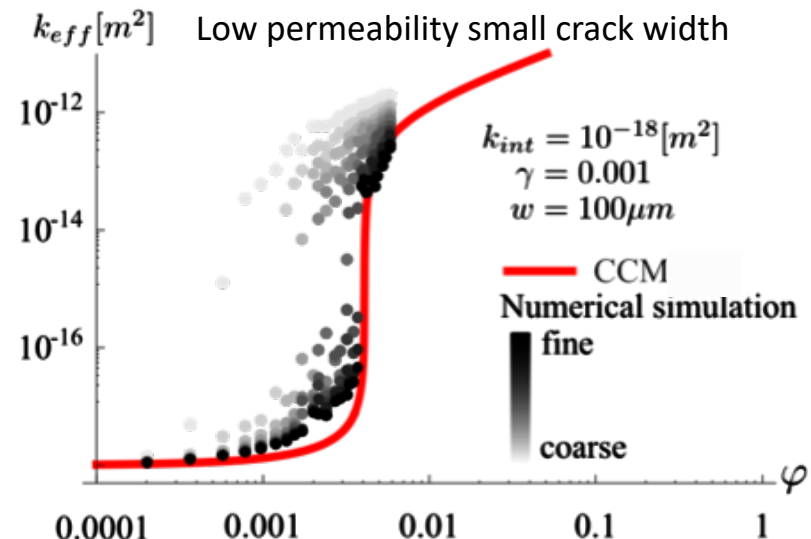
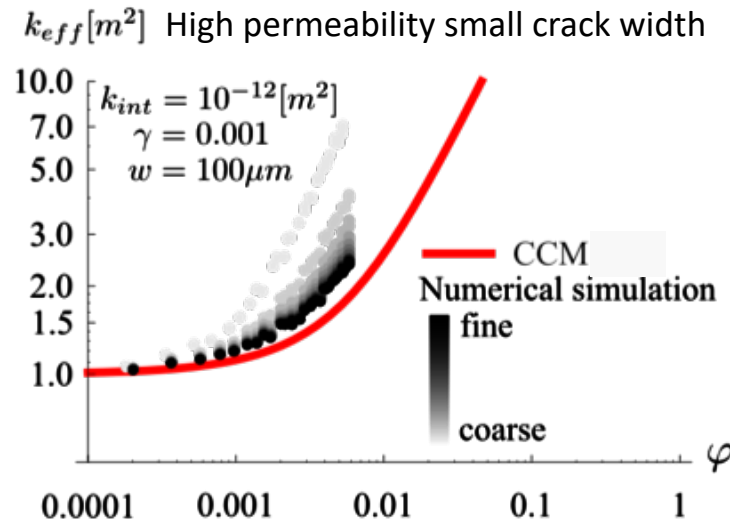
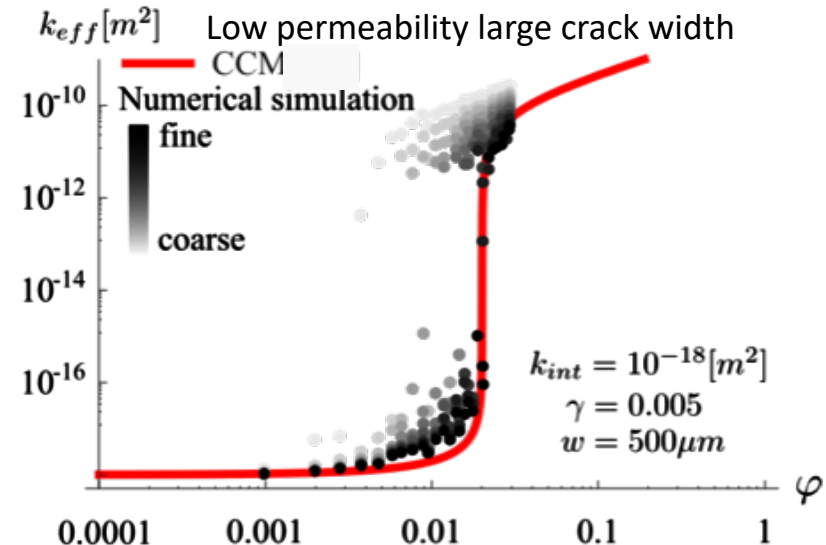
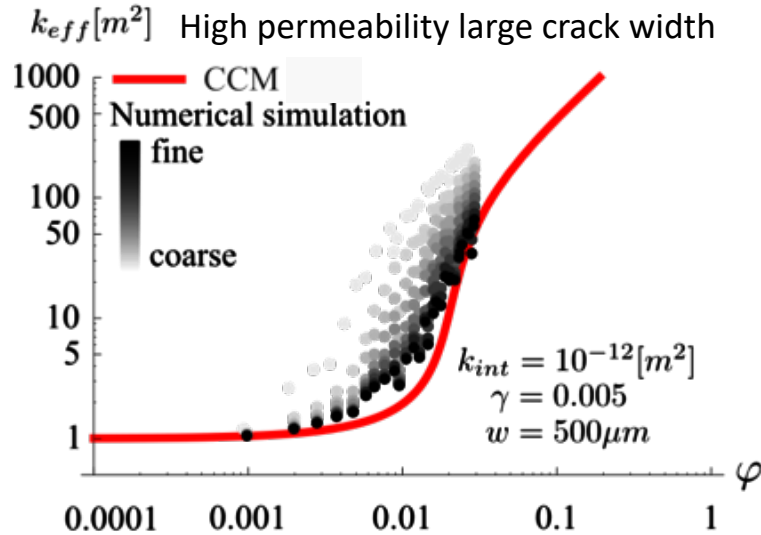
microcrack density

$$\mathbf{k}^e = \mathbf{k}_{int}(1 - \varphi^e) + \mathbf{t}_{\Gamma_c}^T k_c^t(w) \varphi^e \mathbf{t}_{\Gamma_c}$$

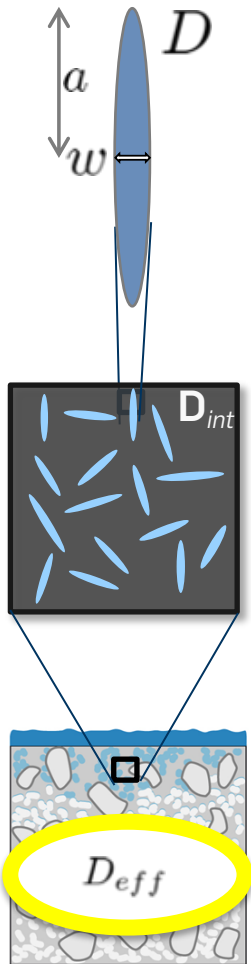
D. Leonhart, J. Timothy & GM (2017) Mechanics of Materials

Effective permeability of cracked porous materials

Computational Meso-scale Analyses vs. Cascade Micromechanics Model



Transient diffusion:



0 microcracks



Isotropic Distribution

100 microcracks



Anisotropic Distribution

100 microcracks



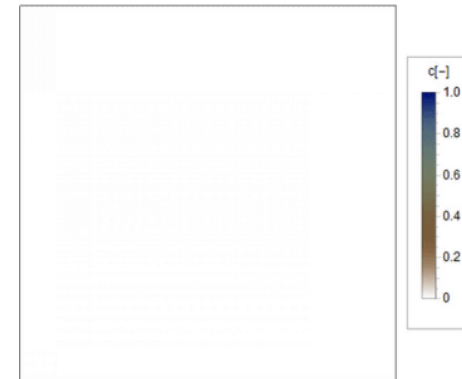
0 microcracks



500 microcracks



500 microcracks

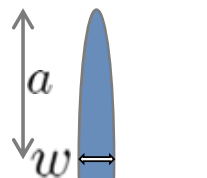


Timothy, J. J. & GM, (2017) Transport in Porous Media, in review

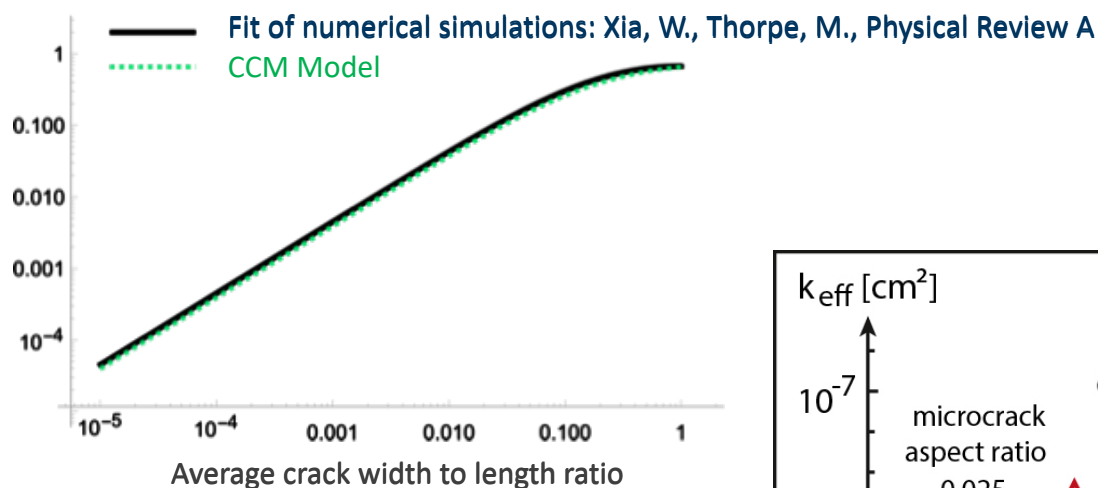
Effective permeability of cracked porous materials

Cascade Continuum Micromechanics Model: Upscaled flux

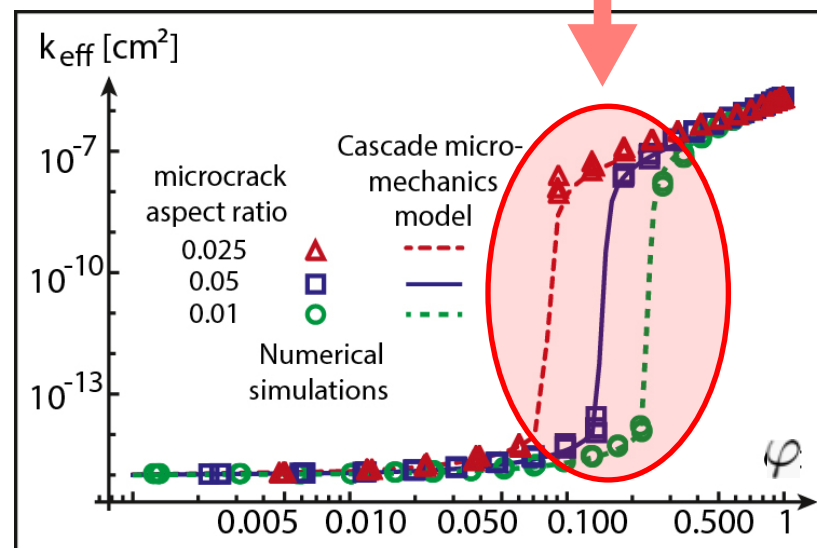
$$\mathbf{k}_{eff}^{(n+1)} = \left(k_{int} (1 - \varphi) \mathbf{A}_{int}^{(n+1)} + k_c \varphi \mathbf{A}_c^{(n+1)} \right) \cdot \mathbf{B}^{(n+1)}$$



Percolation threshold



Power-law relation with aspect ratio of cracks!



Effective permeability: Connected cluster – fractality

At percolation: how does the microcrack cluster look like?

- Pixel update formula (Cellular Automata)

$$p^{t+1}(x, y) = H[p^t(x, y)] + (p_p - 1) H[p^*(x, y) - T]$$

- Moore-Neighbourhood weighting

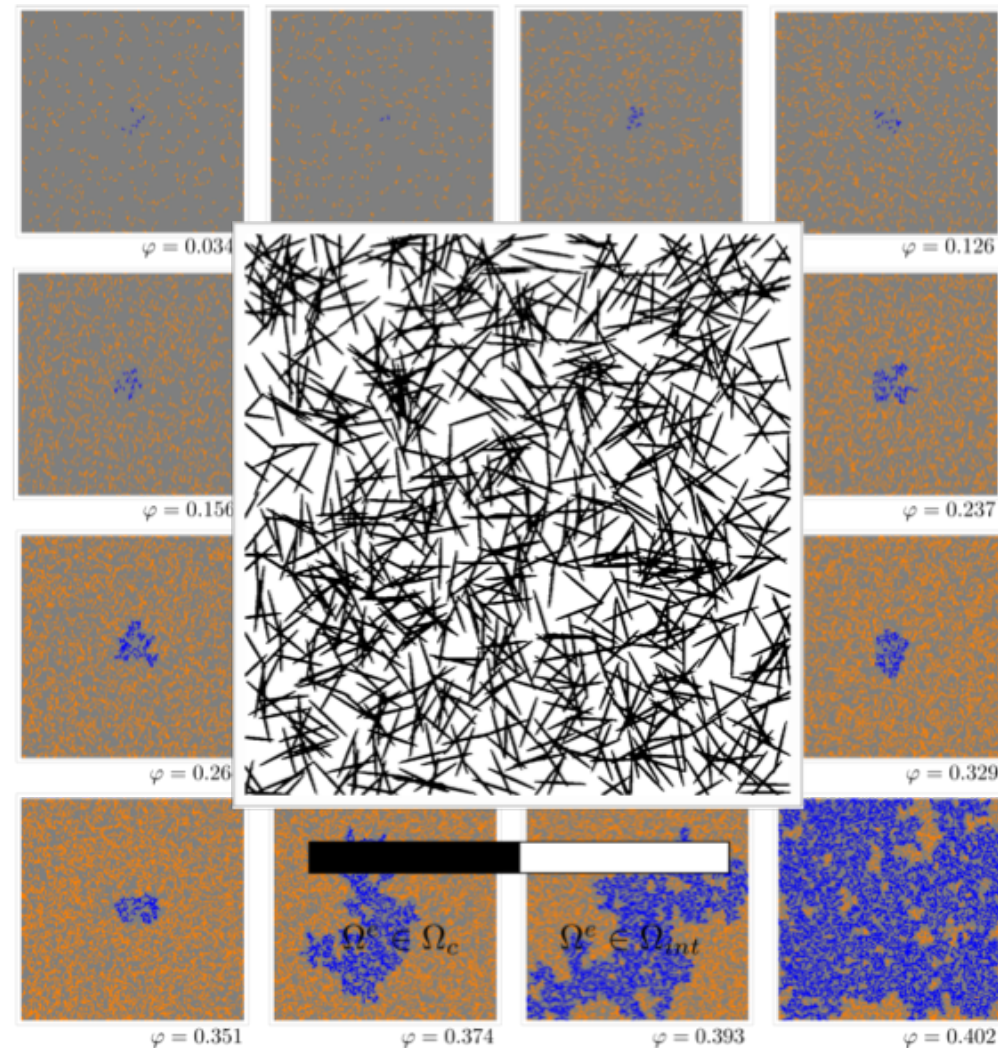
$$p^*(x, y) = \sum_{i=-1}^1 \sum_{j=-1}^1 p^t(x+i, y+j) k(i, j)$$

$$k = \begin{bmatrix} 1 & 1 & 1 \\ 1 & z & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

- Connected microcrack cluster is highly complex with sub-clusters of multiple sizes

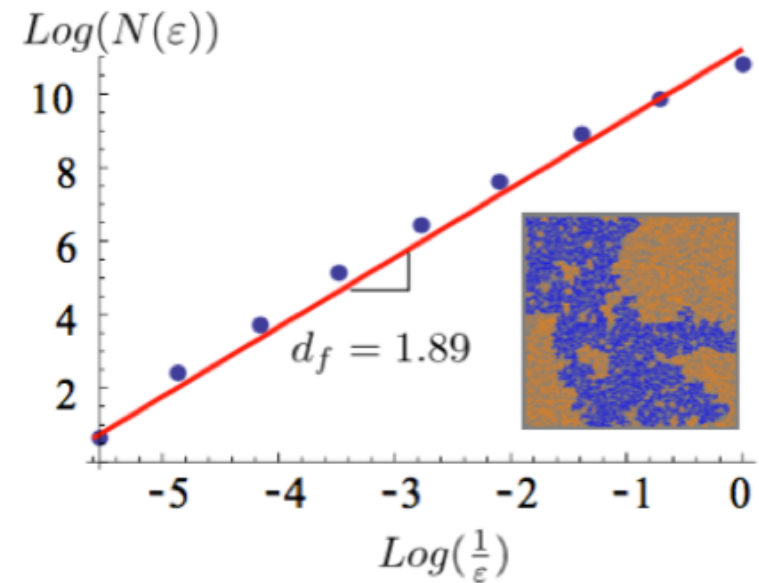
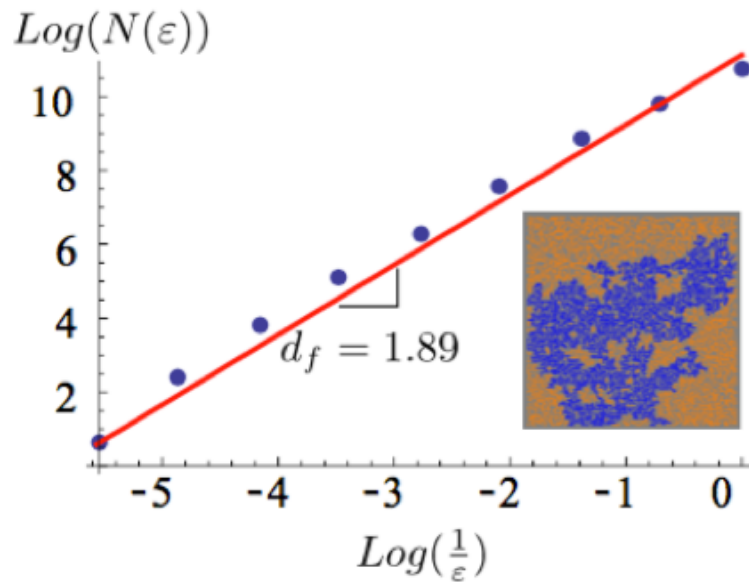
$$\gamma_c = 0.2$$

J.J. Timothy & GM., (2017) Cascade continuum micromechanics model for the effective permeability of solids with distributed microcracks: Self-similar mean-field homogenization and image analysis. *Mechanics of Materials*, 104:60-72.



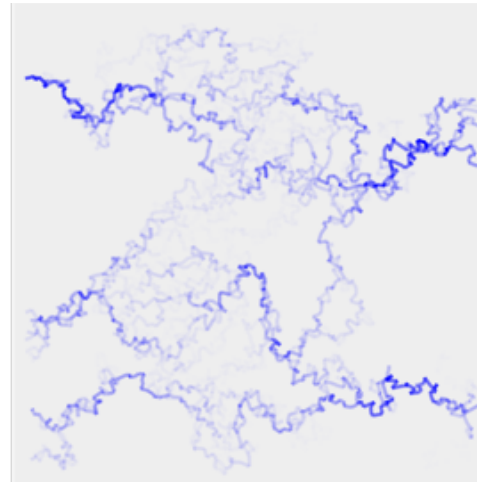
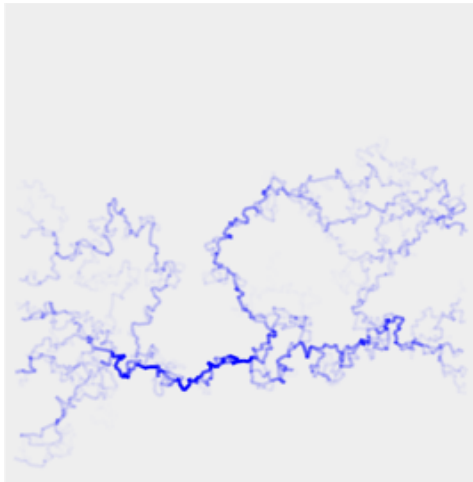
Effective permeability: Connected microcrack cluster – fractality

Fractal dimension around the percolating microcrack cluster (self -similarity):



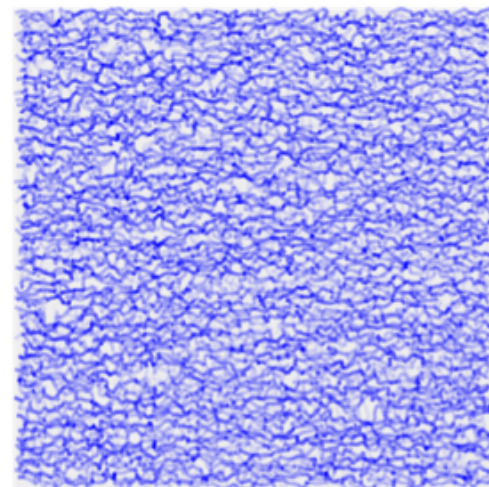
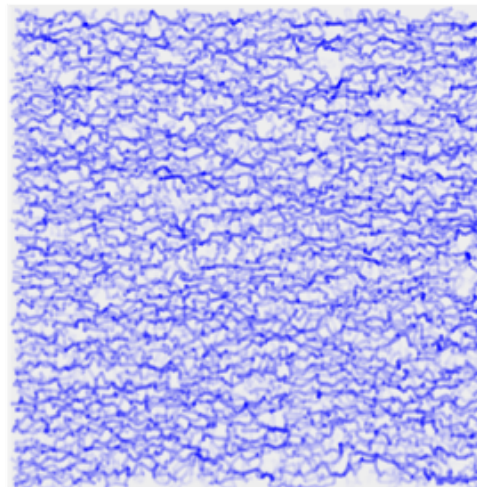
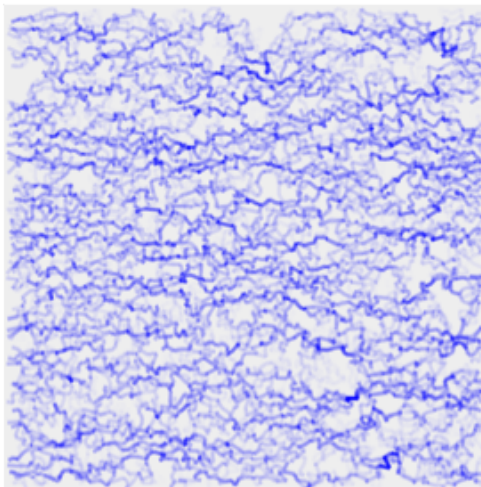
J.J. Timothy & GM (2016) A cascade lattice micromechanics model for the effective permeability of materials with microcracks. *Journal for Nanomechanics and Micromechanics*, 6(4):04016009.

Normalized
fluid flux
around
percolation
threshold



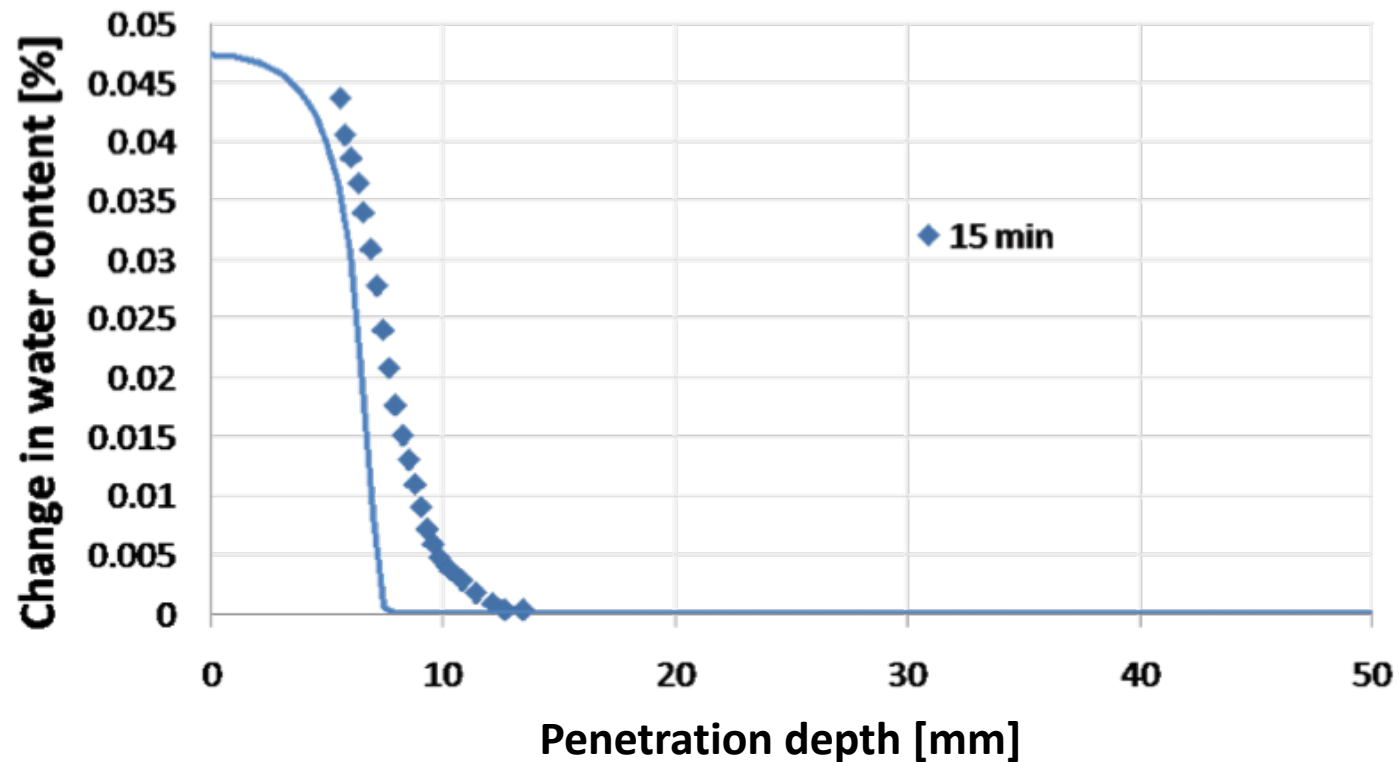
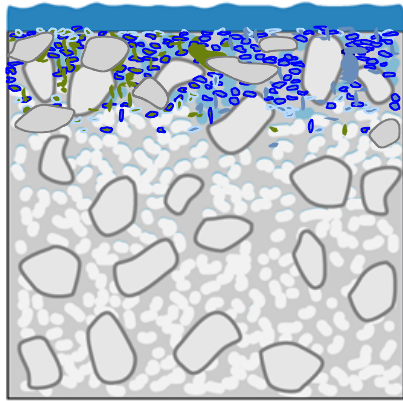
A backbone pathway characterizes the overall transport property

Normalized
fluid flux
above
percolation
threshold



J.J. Timothy & GM (2016) A cascade lattice micromechanics model for the effective permeability of materials with microcracks. *Journal for Nanomechanics and Micromechanics*, 6(4):04016009.

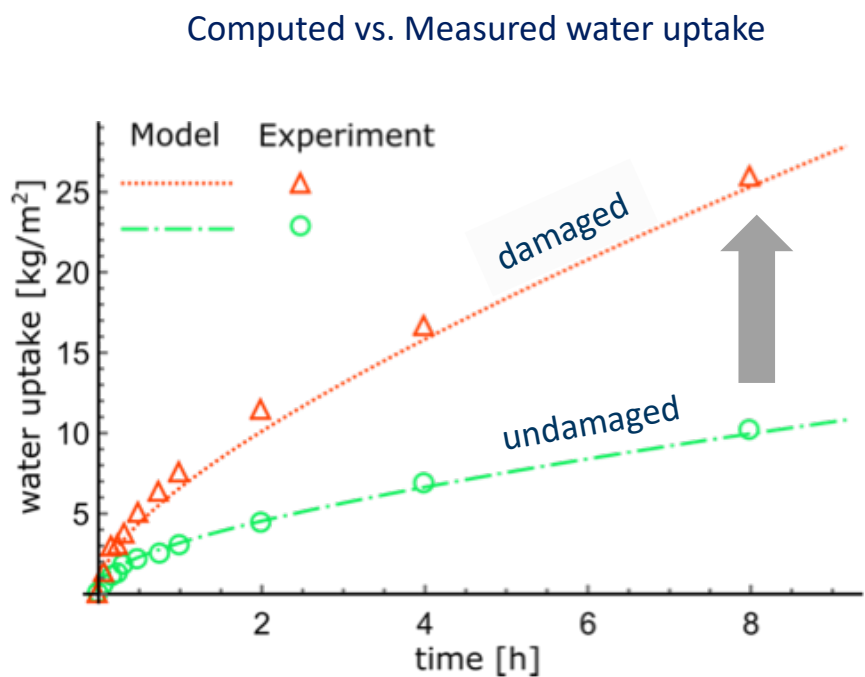
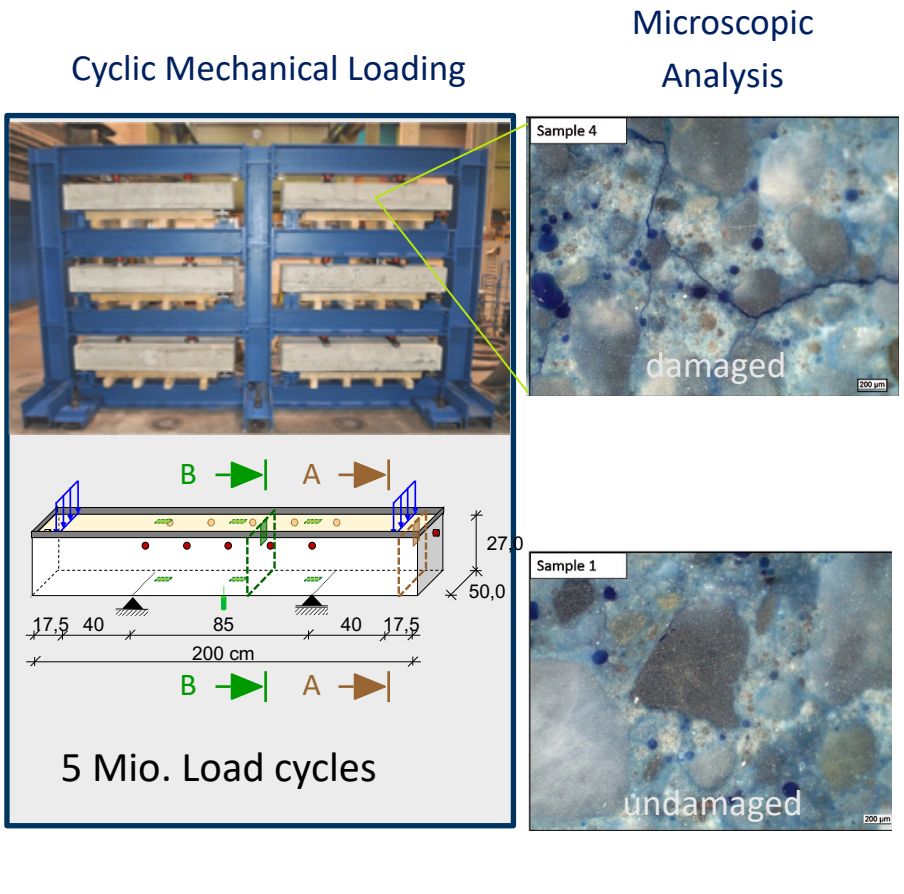
Validation: Capillary suction in intact concrete (not pre-damaged)



Experiments: Zhang, Wittmann, Zhao, Lehmann & Vontobel. Neutron radiography, a powerful method to determine time-dependent moisture distributions in concrete, Nuclear Engineering and Design, 2011

Fluid Transport in Cracked Porous Materials: Experimental Validation

Validation: Capillary suction in pre-damaged concrete

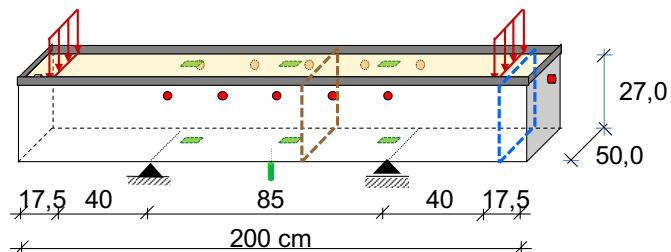


Permeability computed from measured microcrack density from microscopic crack analysis via homogenization

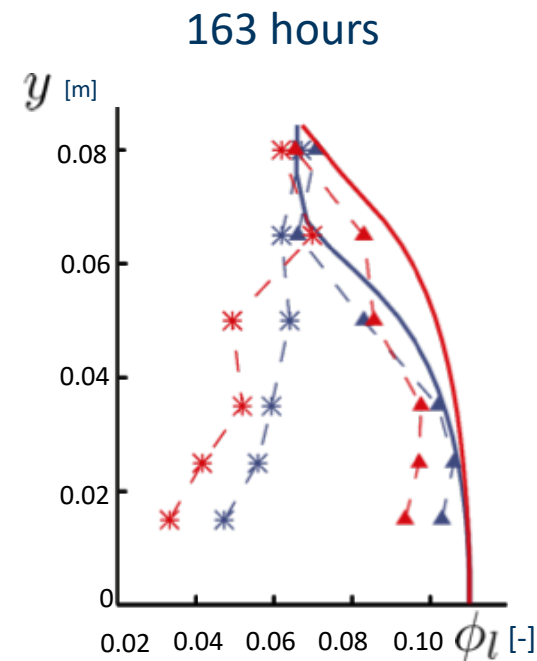
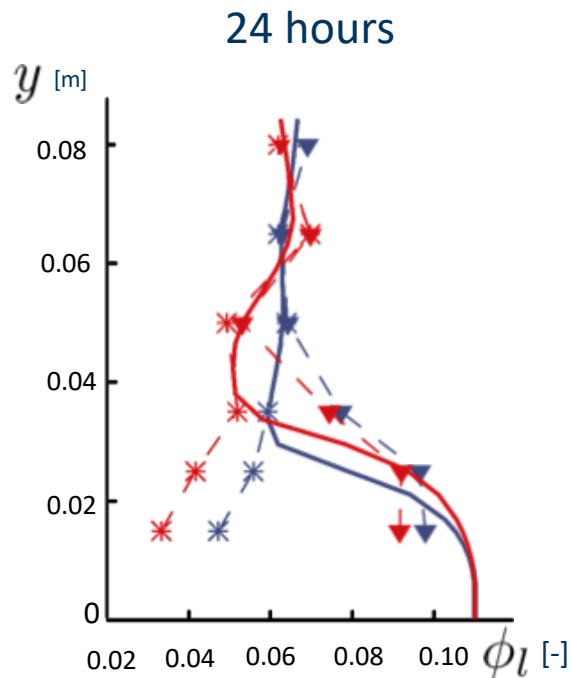
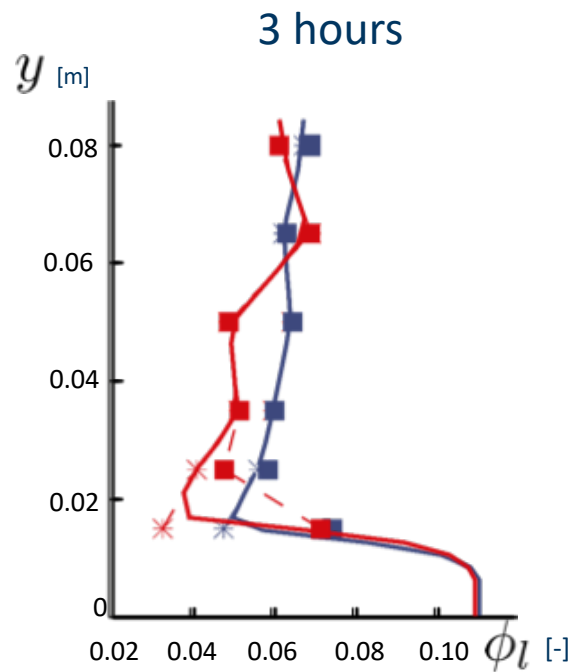
Przondziona, R., Timothy, J. J., M., Weise, Krutt, E., F., Breitenbücher, R., GM & Hofmann, M. (2017). Degradation in concrete structures due to cyclic loading and its effect on transport processes - Experiments and Modelling. *Structural Concrete*

Fluid Transport in cracked concrete: Experimental Validation

Influence of diffuse fatigue cracks on water transport

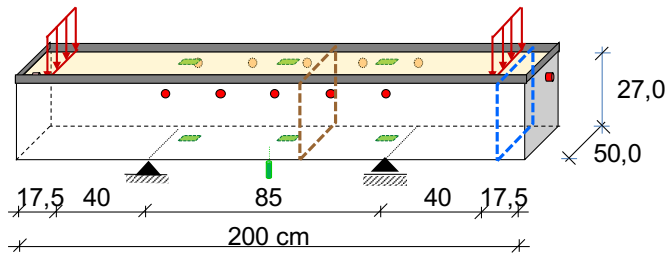


	Experiment	Model
Intact concrete	* ■ ▼ ▲	—
Cracked concrete	* ■ ▼ ▲	—

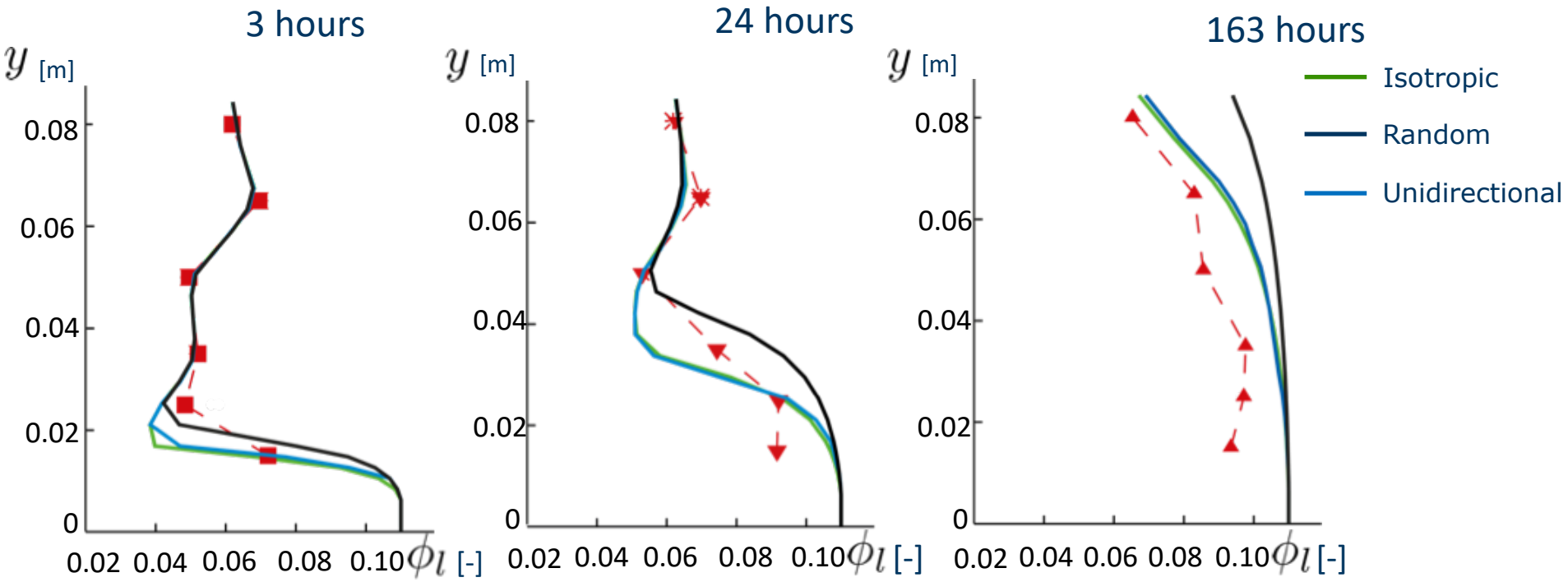


TDR Messungen: BAM – FOR 1498, TP 4, siehe Weise, Meng et al. IBAUSIL 2011

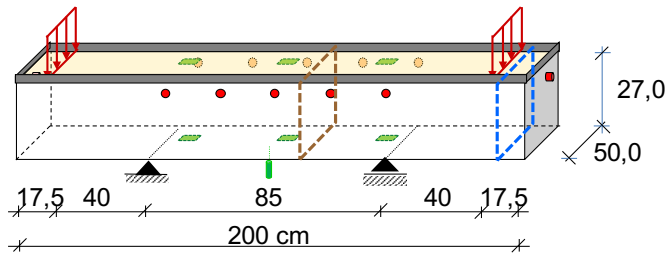
Influence of crack topology



	Experiment	Model
Cracked concrete	* ■ ▼ ▲	— — —



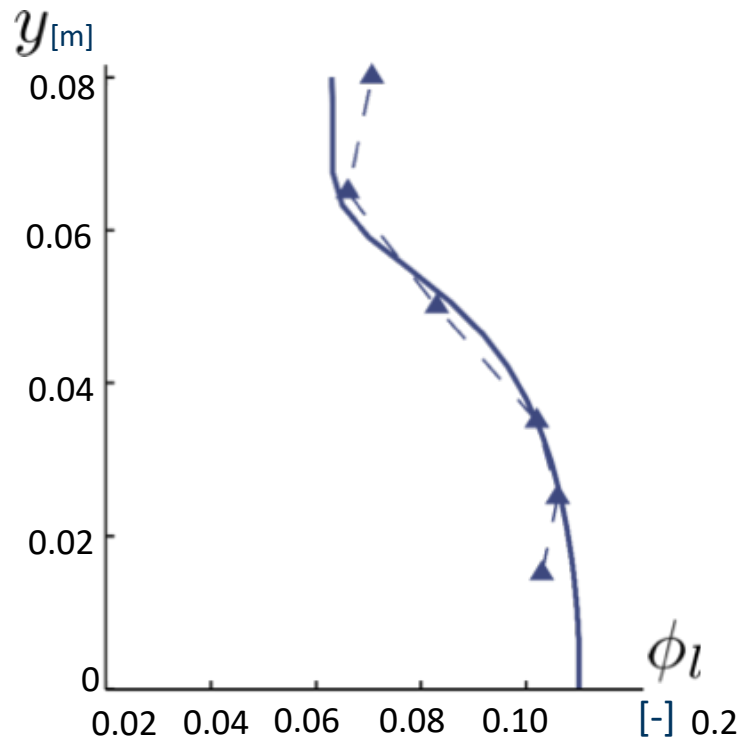
TDR Measurements: BAM 2015



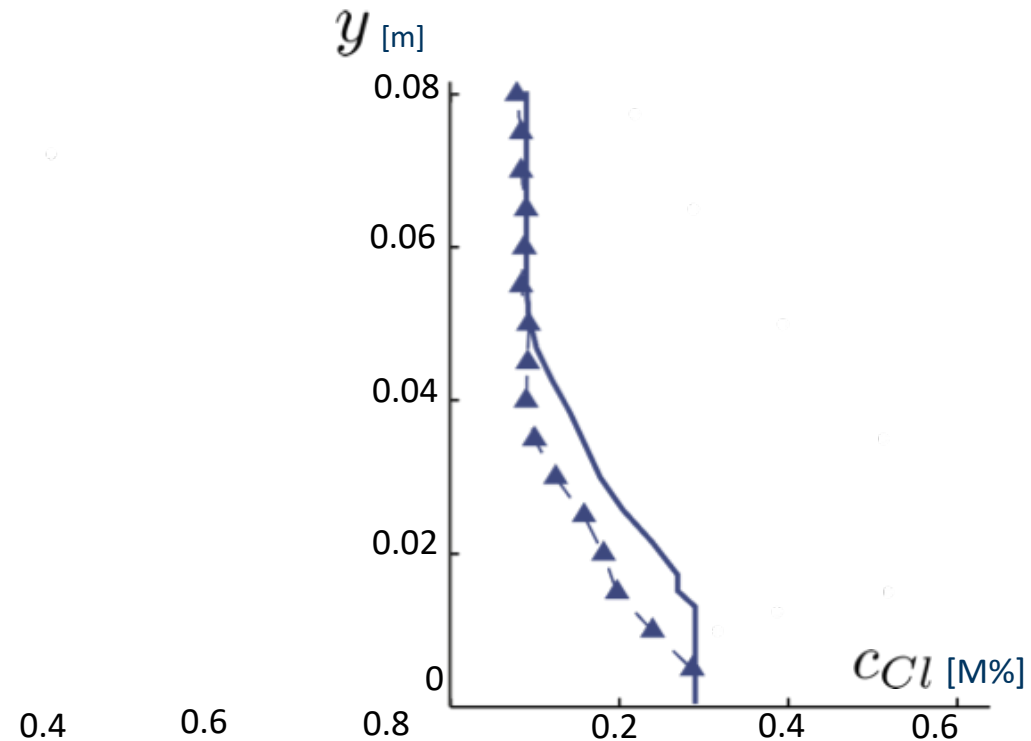
Experiment Model



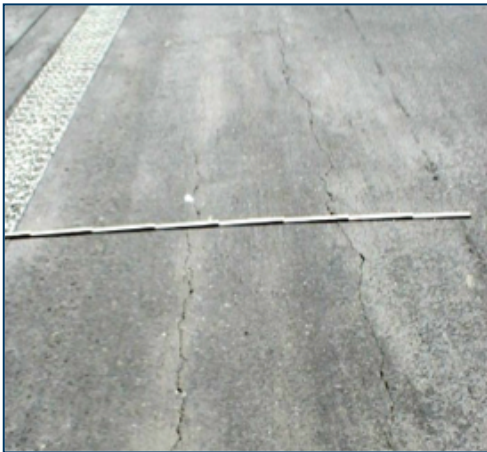
Fluid transport after 163 hours



Cl- ion profile after 163 hours



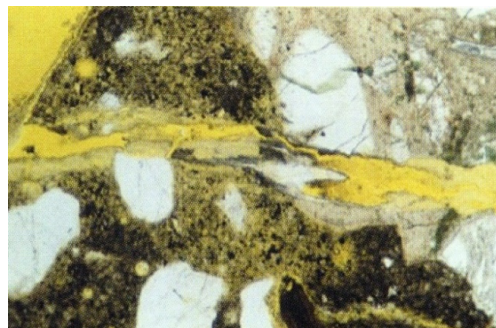
Messungen: BAM 2016



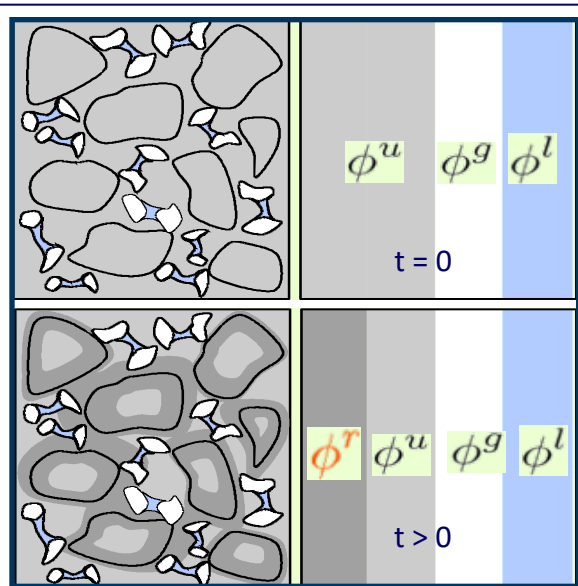
- Chemical reaction between silica (SiO_2) in aggregates and alkali hydroxides in pore solution results in formation of a gel
- Gel swells by imbibition of water and exerts pressure on skeleton
- Reaction rate and level depends on moisture content



- Consequences:
- Macroscopic expansion
- Opening and propagation of cracks
- Reduction of stiffness and load carrying capacity



STARK & WICHT 2000



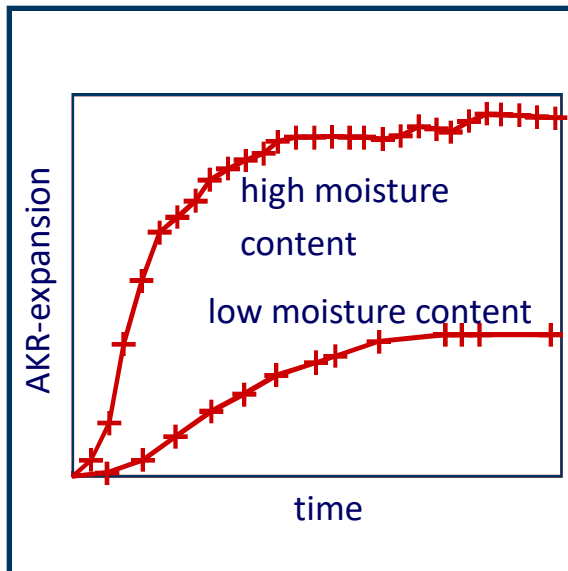
Solid skeleton φ^s $\left\{ \begin{array}{l} \text{Unreacted, unswollen constituent } \varphi^u \\ \text{Reacted, swollen constituent } \varphi^r \end{array} \right.$

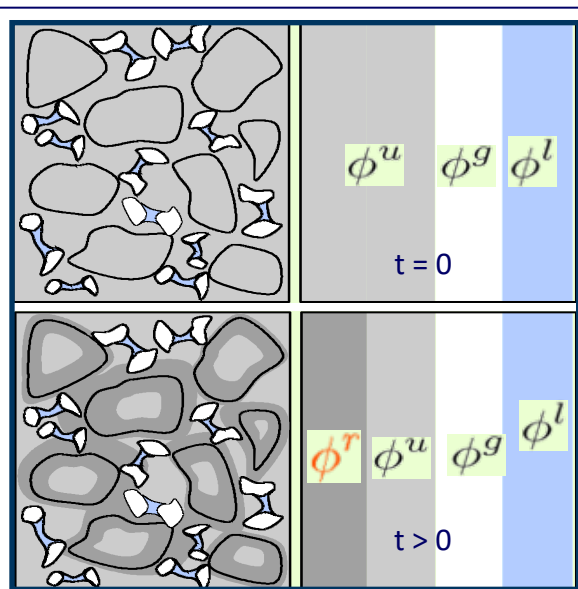
mass exchange between unreacted and reacted phase

$$\varrho^u \frac{\partial \phi^u}{\partial t} = \varrho^u \frac{\partial \phi^{u \rightarrow r}}{\partial t} \quad \varrho^r \frac{\partial \phi^r}{\partial t} = \varrho^r \frac{\partial \phi^{r \leftarrow u}}{\partial t}$$

1st order kinetic law: $\varrho^u \frac{\partial \phi^{u \rightarrow r}}{\partial t} = -\frac{1}{\tau(S_l)} \varrho^u \phi^u$

$\frac{1}{\tau(S_l)}$: reaction velocity: depends on S_l





Solid skeleton φ^s $\begin{cases} \text{Unreacted, unswollen constituent } \varphi^u \\ \text{Reacted, swollen constituent } \varphi^r \end{cases}$

mass exchange between unreacted and reacted phase

$$\varrho^u \frac{\partial \phi^u}{\partial t} = \varrho^u \frac{\partial \phi^{u \rightarrow r}}{\partial t} \quad \varrho^r \frac{\partial \phi^r}{\partial t} = \varrho^r \frac{\partial \phi^{r \leftarrow u}}{\partial t}$$

1st order kinetic law: $\varrho^u \frac{\partial \phi^{u \rightarrow r}}{\partial t} = -\frac{1}{\tau(S_l)} \varrho^u \phi^u$

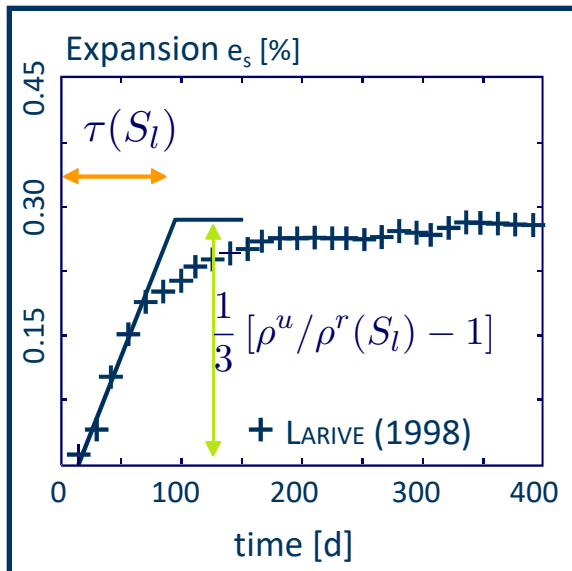
$\frac{1}{\tau(S_l)}$: reaction velocity: depends on S_l

Macroscopic ASR expansion: $\varepsilon_s^a = \frac{1}{3} \left[\frac{\varrho^u}{\varrho^r} - 1 \right] \xi$

Reaction degree: $\xi = 1 - e^{-t/\tau}$

Effective density: $\varrho^s = \frac{\varrho^u \varrho^r}{\varrho^r + \xi[\varrho^u - \varrho^r]}$

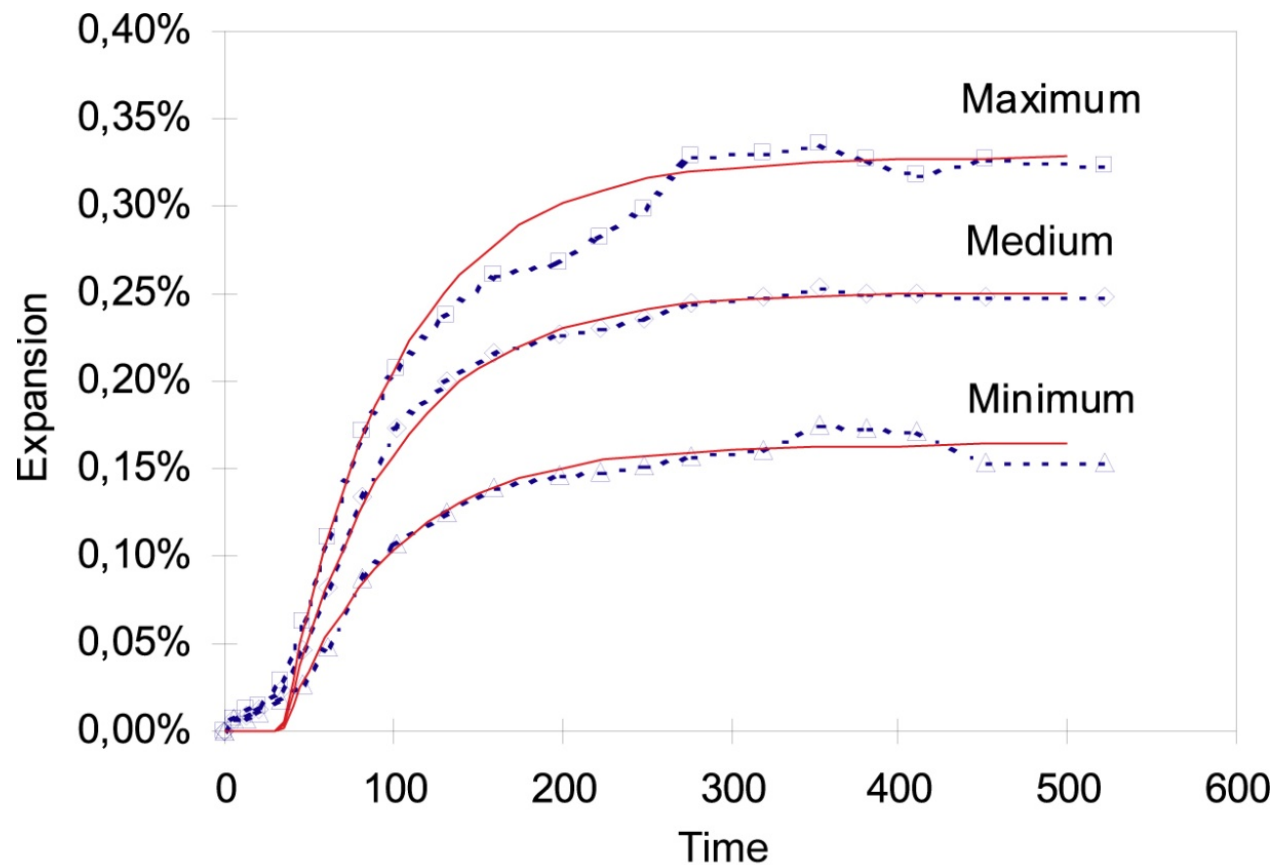
Gradient enhanced isotropic damage model



Bangert, F.; Grasberger, S.; Kuhl, D. & GM (2003), Engineering Fracture Mechanics

Bangert, F.; Kuhl, D. & GM (2004), Int. J. Numerical and Analytical Methods in Geomechanics

Calibration of ASR model [MULTON 2003, POYET 2003]

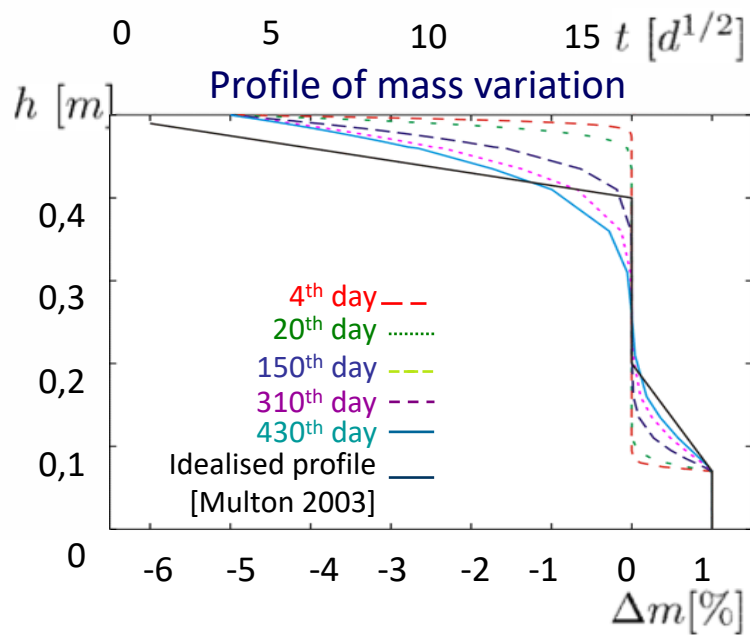
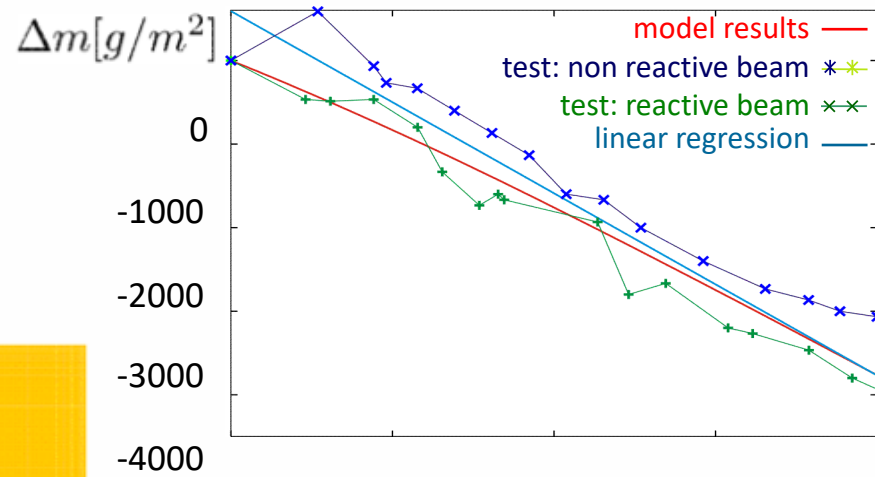
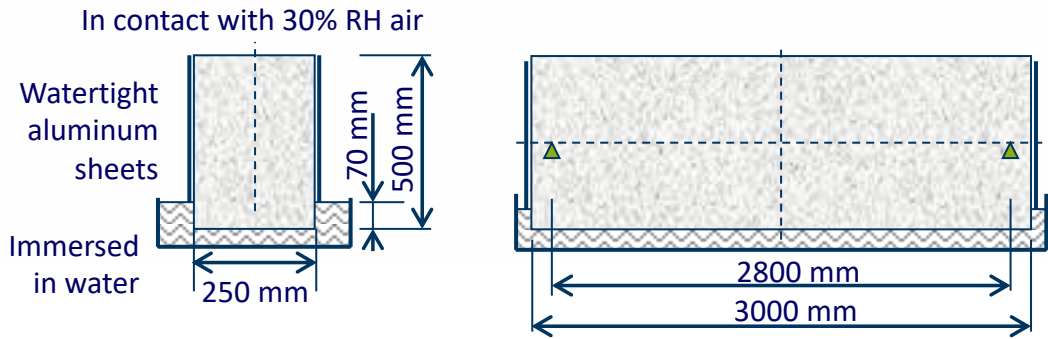
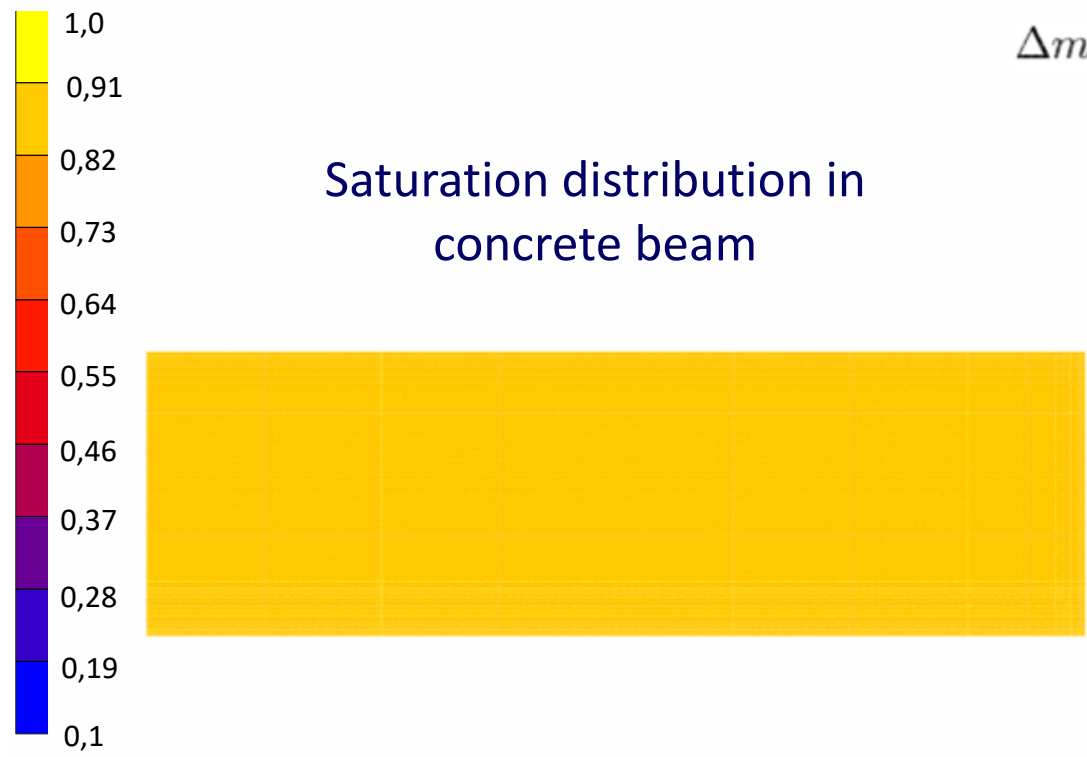


Bangert, F.; Grasberger, S.; Kuhl, D. & GM (2003), Engineering Fracture Mechanics

Bangert, F.; Kuhl, D. & GM (2004), International Journal for Numerical and Analytical Methods in Geomechanics

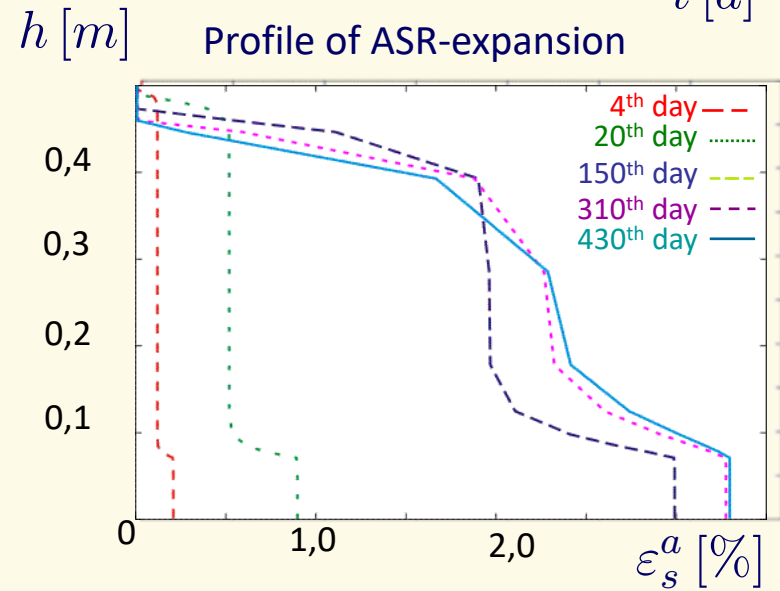
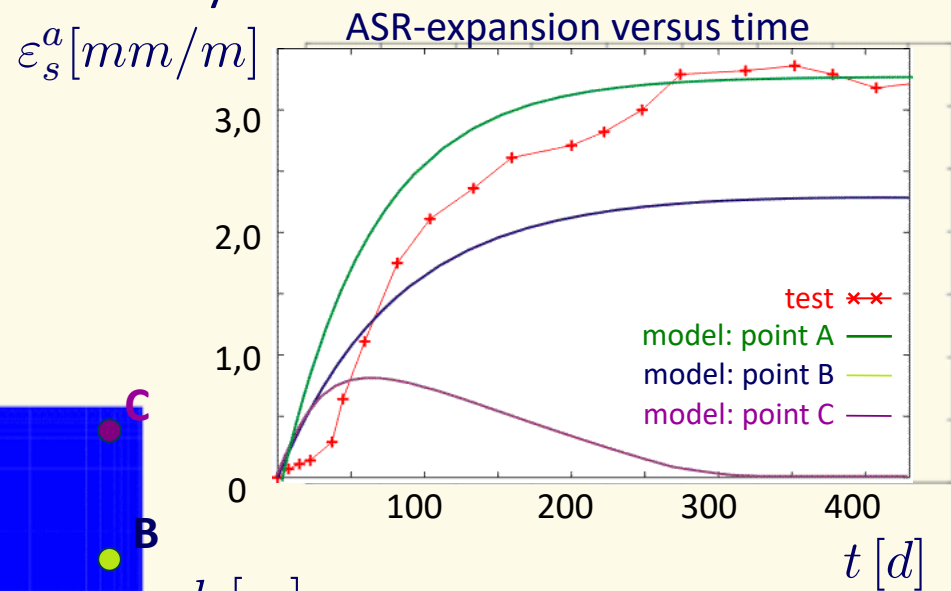
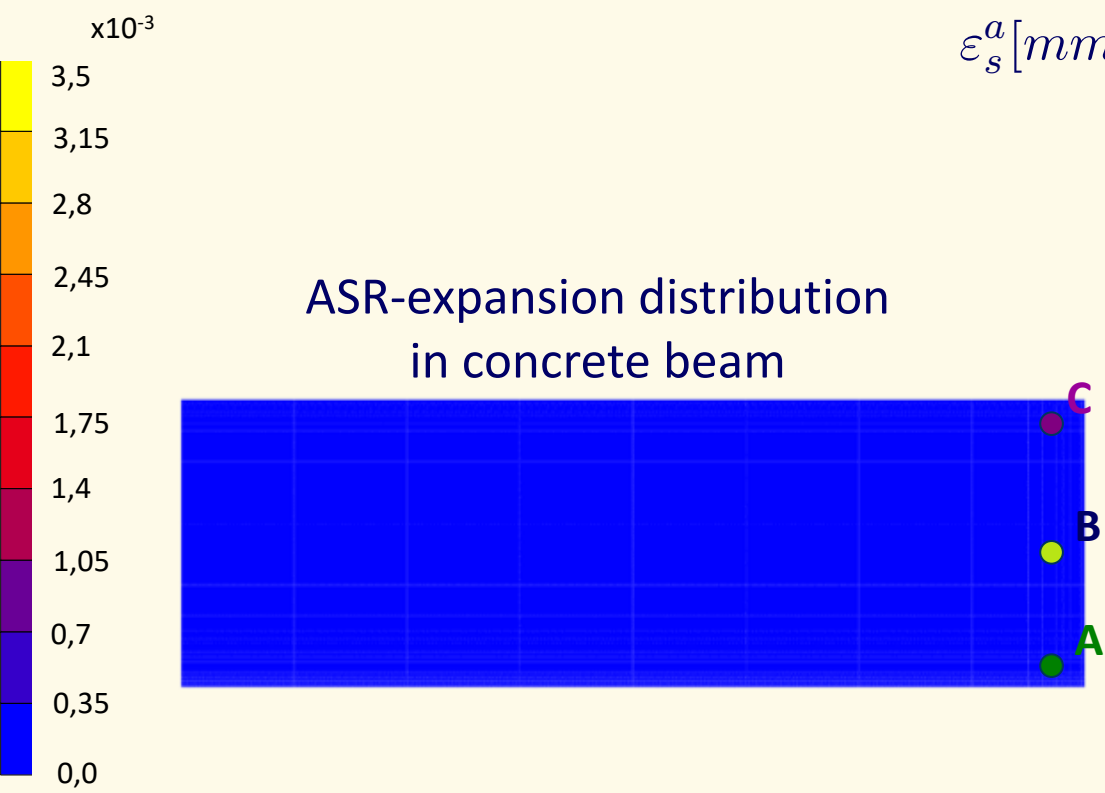
Phenomenological model of ASR-induced deterioration in concrete

Numerical simulation of a concrete beam affected by ASR



Phenomenological model of ASR-induced deterioration in concrete

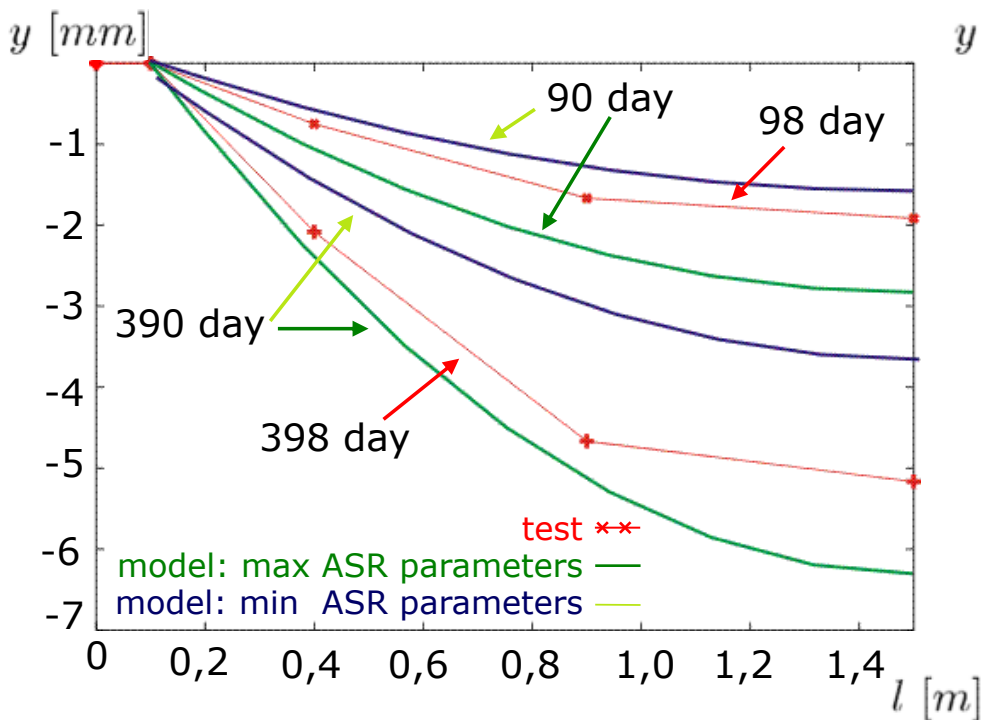
Numerical simulation of a concrete beam affected by ASR



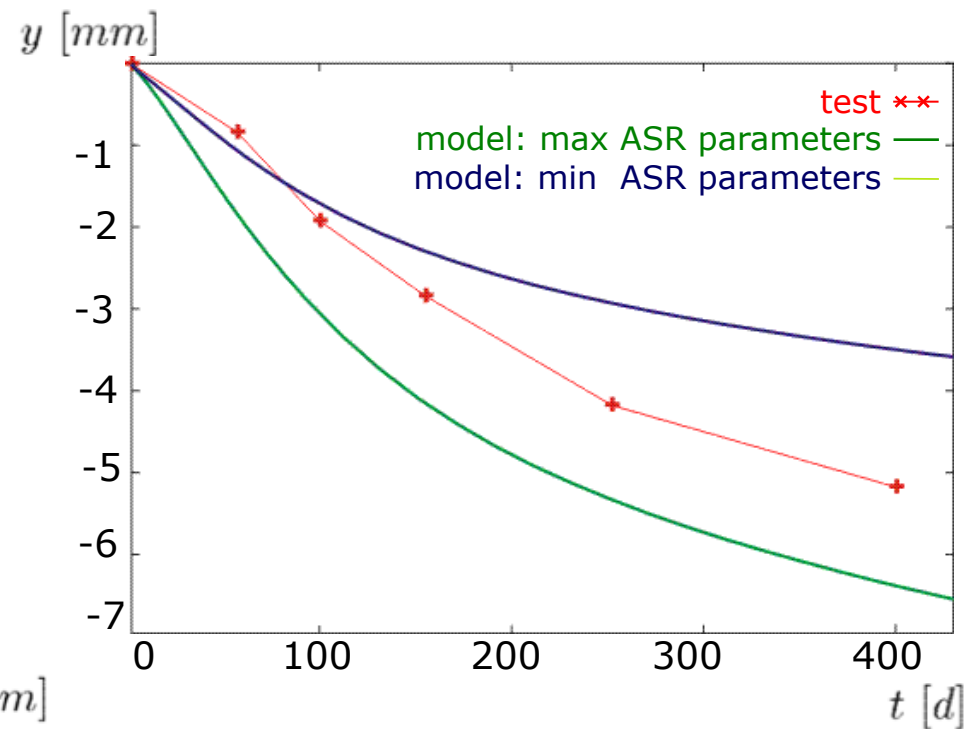
Phenomenological model of ASR-induced deterioration in concrete

Numerical simulation of a concrete beam affected by ASR

Deflection along length of beam



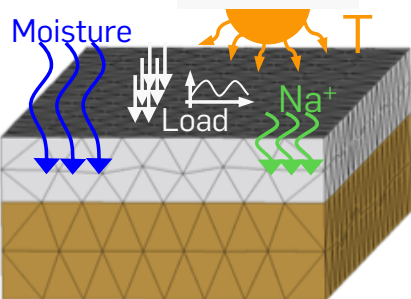
Maximal deflection versus time



Macroscale [m]



Durability Analysis

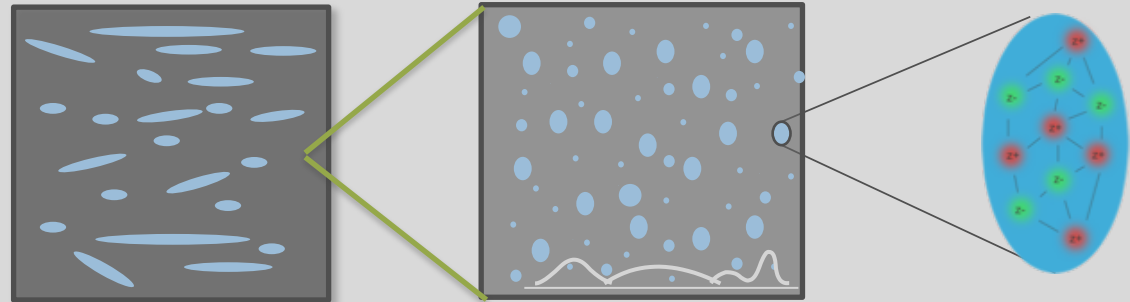


Finite Element Model

Macroscopic Laws

Multiscale model for Alkali and fluid transport (nm - mm)

Transport



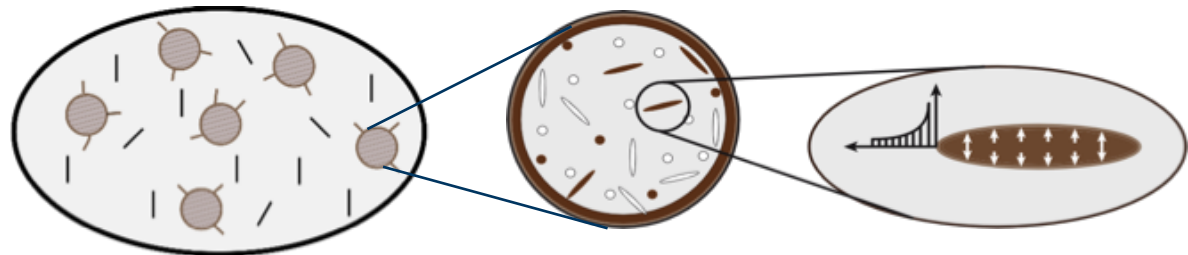
Microcracks

Pore Space

Pore fluid

Multiscale model for damage (μm - cm)

Deterioration

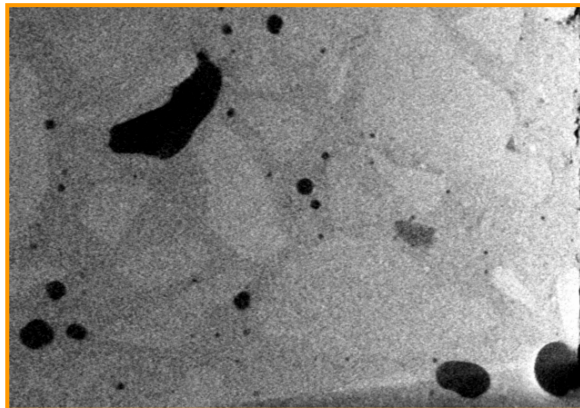


Concrete

Aggregates

Microcracks

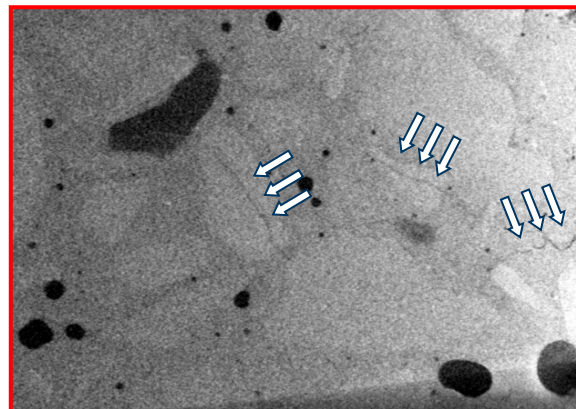
No microcracking observed



t = 0

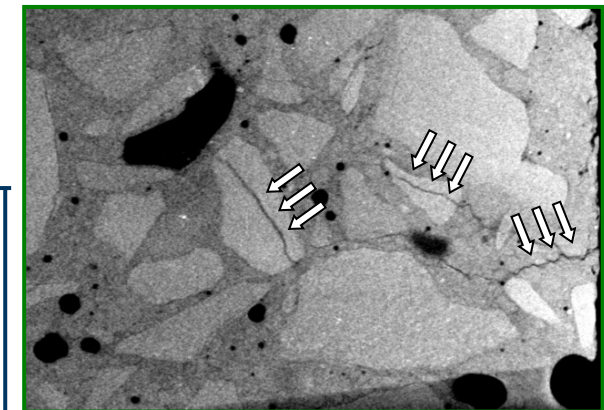
Experimentally observed ASR-induced microcracking (3D-CT)

Microcracks in aggregates



t = 2 months

Crack propagation into cement paste

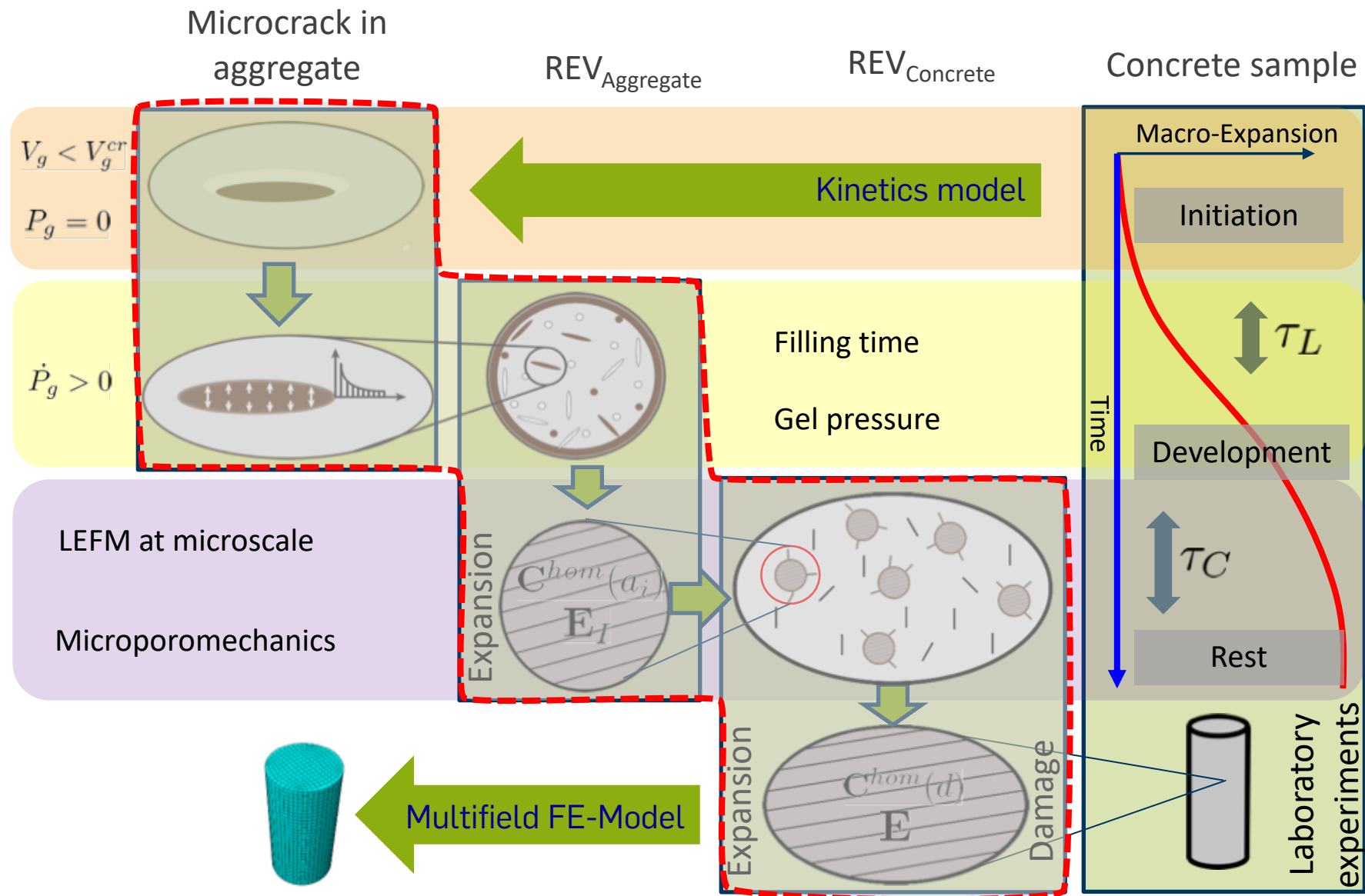


t = 5 months

10 mm

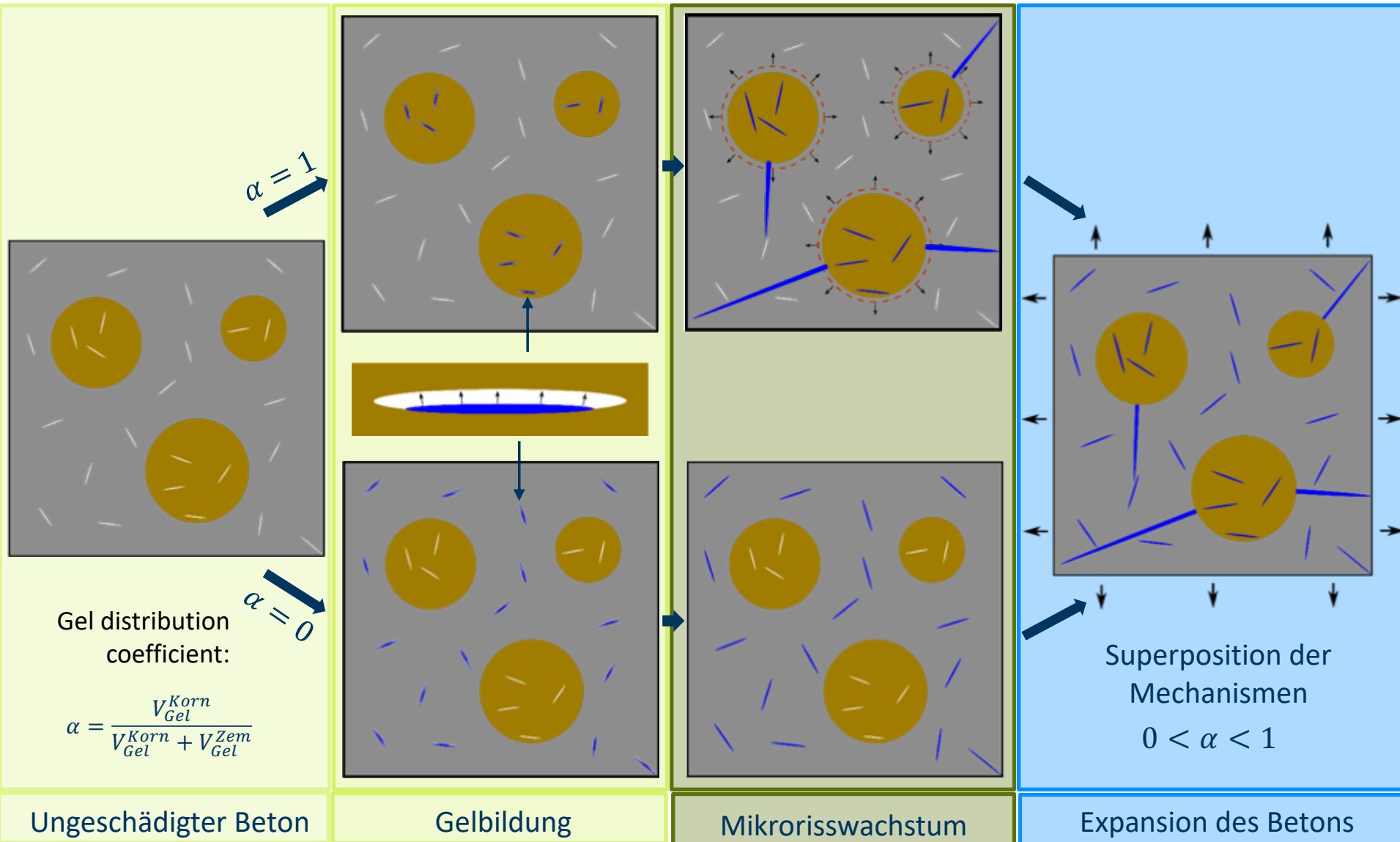
Weise, 2016: BAM (Federal Institute for Materials Research and Testing)

ASR-Expansion in concrete: A multiscale problem

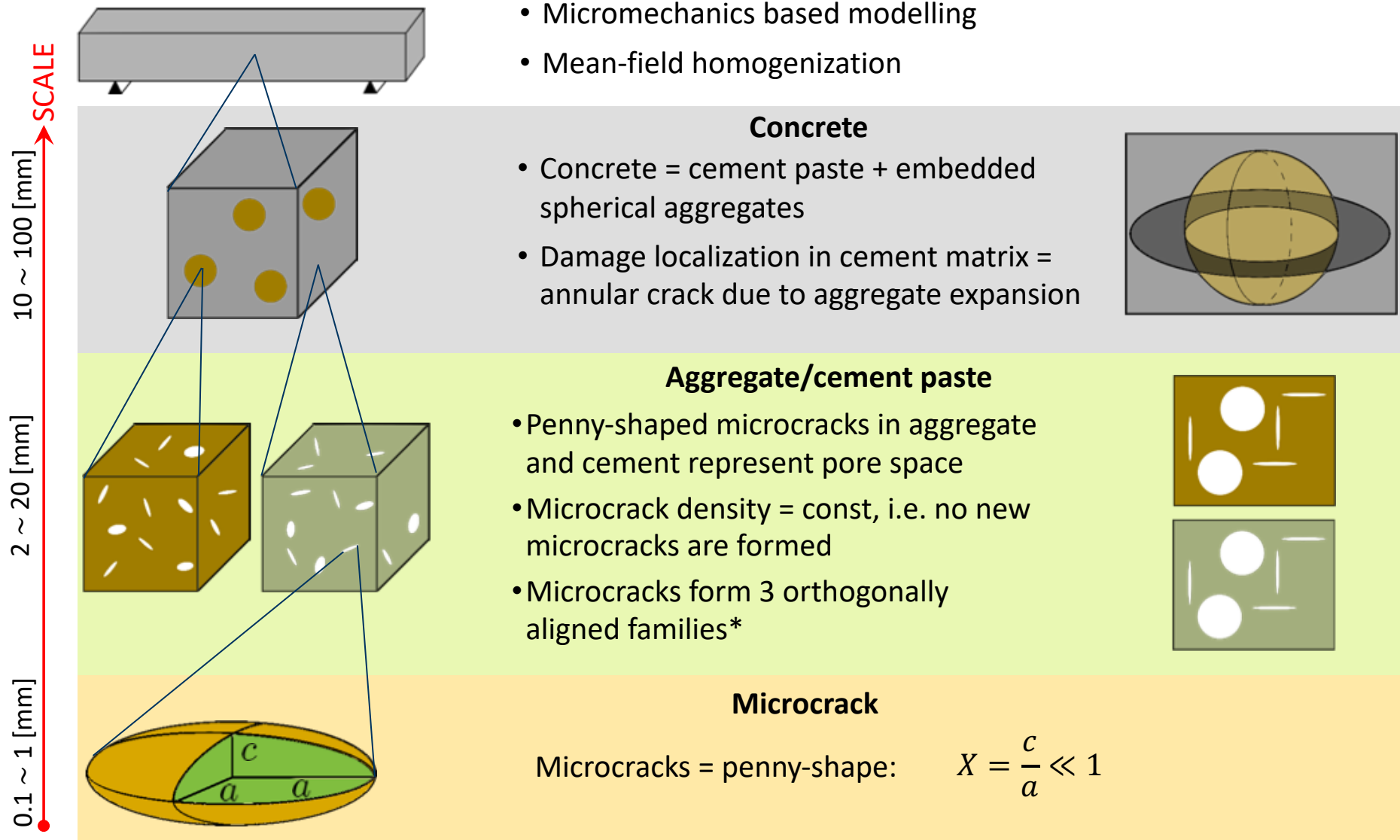


ASR-Expansion in concrete: a multiscale problem

Macroscopic expansion and damage: upscaling of microcrack propagation



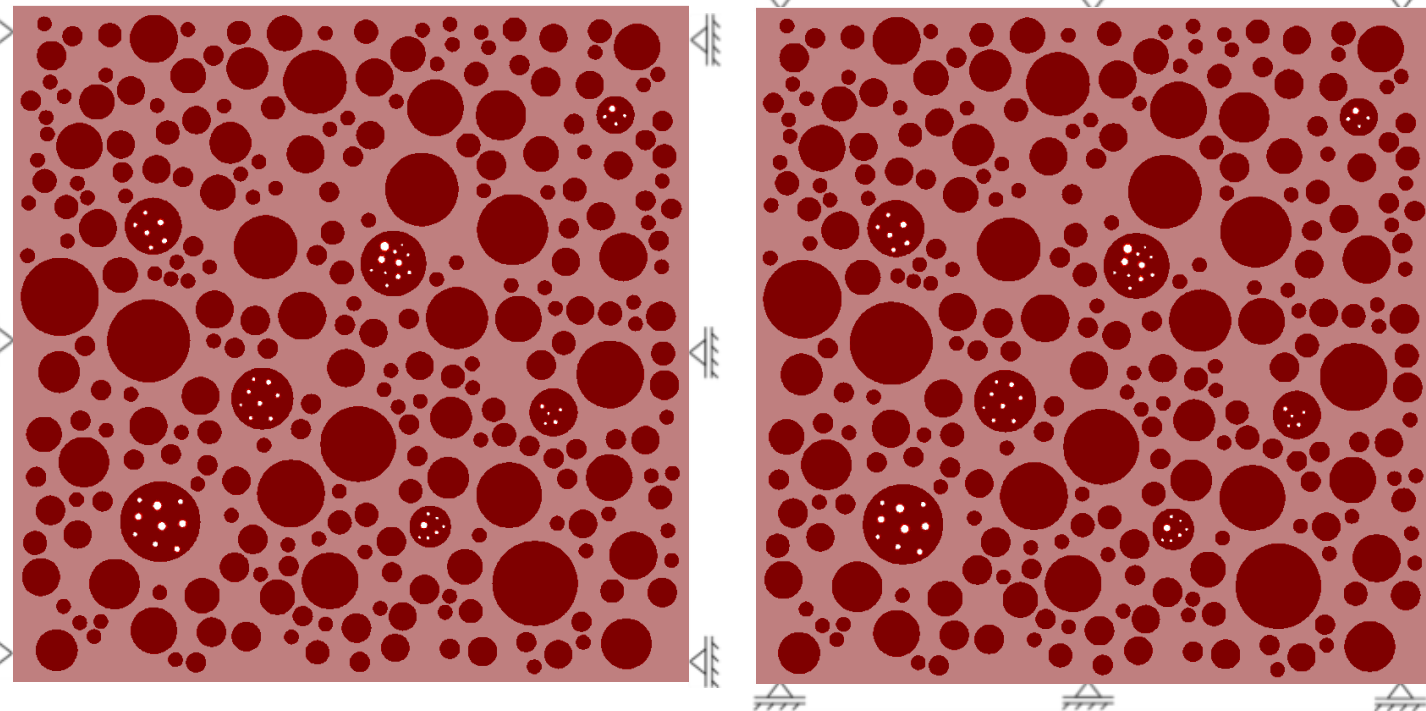
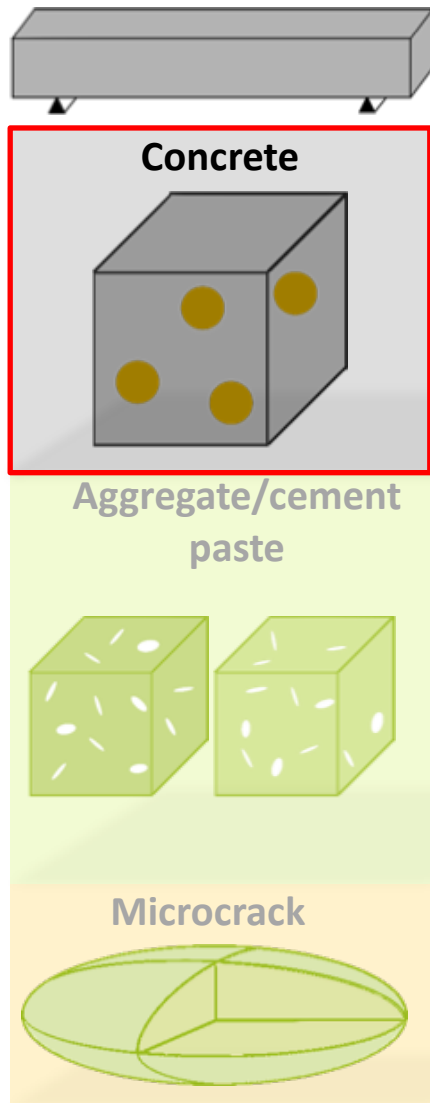
ASR-Expansion in concrete: a multiscale problem



* Charpin & Ehrlacher 2012, Esposito, 2016, Ph.D. thesis

Cracking due to pressure in gel pockets in aggregates: mesostructure simulation of horizontal and vertically constrained expansion

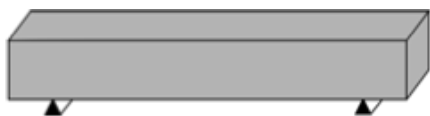
Crack propagation simulation: Variational Interface fracture model*



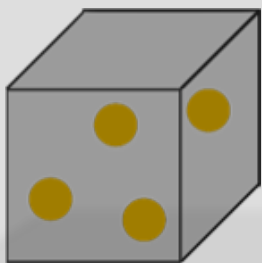
- Cracks initiate within the aggregate, propagate and coalesce
- After cracks reach the cement, they propagate into cement paste, forming ring-shaped cracks
- Formation of **radial cracks in cement paste** -> **Annular crack concept**

I. Khisamitov & GM, CMAME, submitted 2017

ASR-Expansion: Combine micromechanics with fracture mechanics



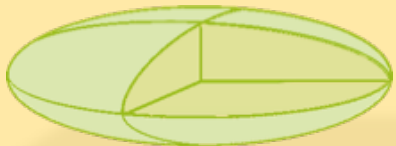
Concrete



Aggregate/cement paste

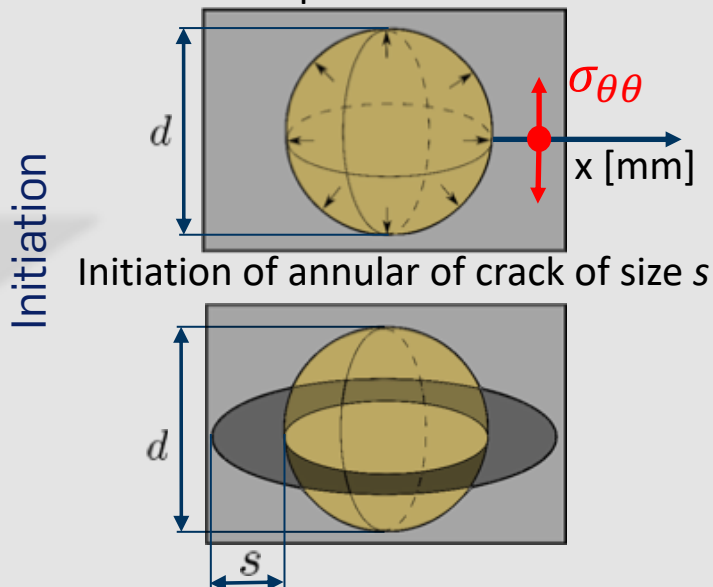


Microcrack

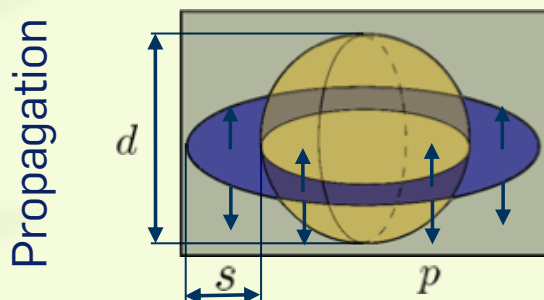


Annular crack around the aggregate

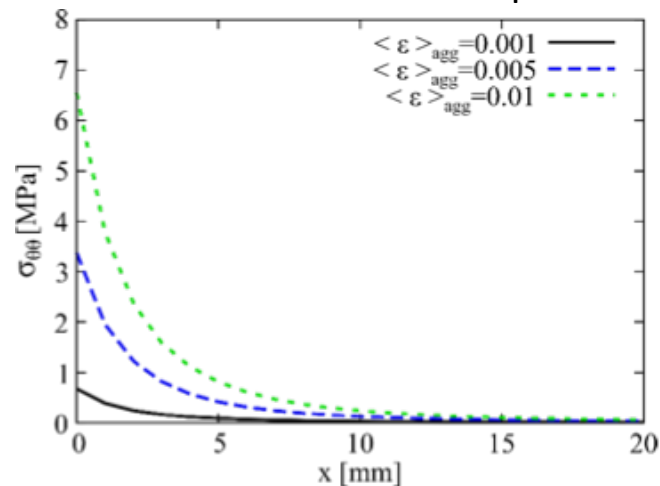
Aggregate expansion $\rightarrow$ tensile stresses in cement paste around it



Annular crack growth due to gel pressure



Tensile stress in cement paste



(using exterior point Eshelby tensor)

Ju & Sun, 1999

Annular crack formation criterion:

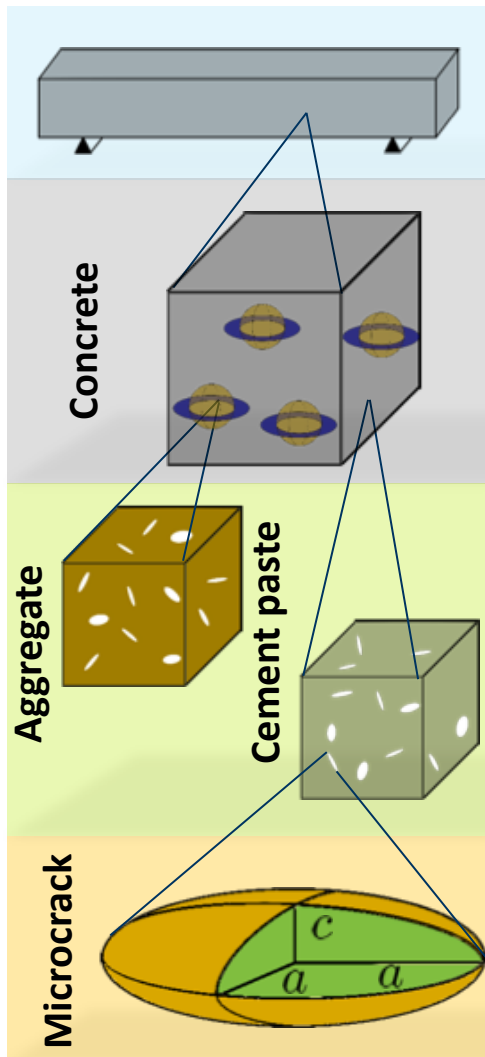
$$K_I(s) - K_{Ic} \leq 0$$

$$K_I(s) = \int_0^s h(x, s, d) \sigma_{\theta\theta}(x) dx$$

Fett & Rizzi, 2007, Forschungszentrum Karlsruhe

ASR-Expansion in concrete: a multiscale problem

Macroscopic damage: upscaling of microcrack propagation



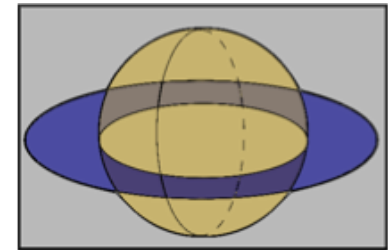
Macroscopic expansion and damage

$$\mathbb{C}_{macro}^{hom}, \mathbf{E}_{macro}$$

Annular crack initiation and propagation

$$\sigma_{\theta\theta} = f(\mathbf{E}_{agg}, \mathbb{C}_{agg}^{hom}, \mathbb{C}_{cem}^{hom})$$

$$K_I(\sigma_{\theta\theta}) - K_{Ic} \leq 0$$



Aggregate expansion due to microcracking

$$G(a, \Sigma, p) = \frac{\partial \Psi(\phi_c, \Sigma, p)}{\partial \phi_c} \leq G^c$$

pressure p at which microcrack starts propagating $\rightarrow$ aggregate expansion

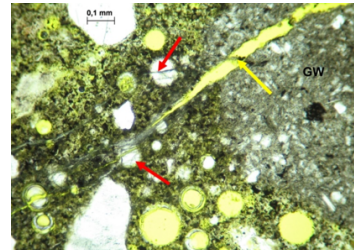
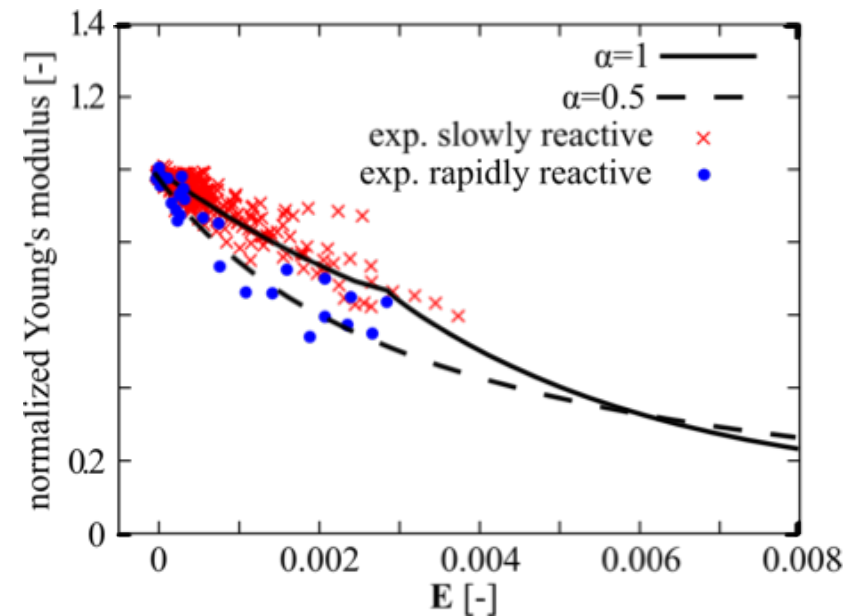
Growth of penny shaped microcracks in aggregates

$$\begin{cases} G(a, \Sigma, p) - G_c \leq 0 \\ \dot{a} \geq 0 \\ (G(a, \Sigma, p) - G_c) \dot{a} = 0 \end{cases}$$

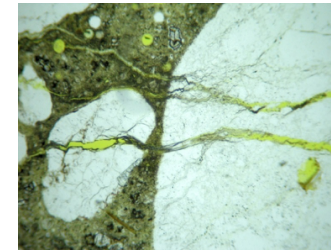
ASR expansion of concrete: Comparison with experimental data

Elastizitätsmodul vs. freie Expansion

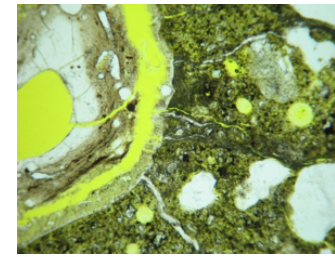
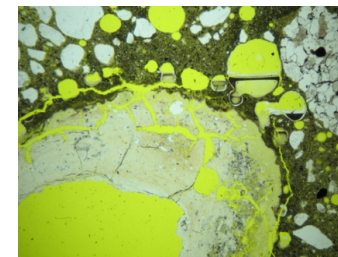
Vergleich mit experimentellen Daten (Giebson, 2013)



$\alpha = 1$: Microcracking begins in the aggregate and propagates into the cement paste



Slowly reactive
(Giebson, 2013)



Rapidly reactive
(Giebson, 2013)

$\alpha = 0.5$: Microcracking begins in the cement paste and aggregate simultaneously

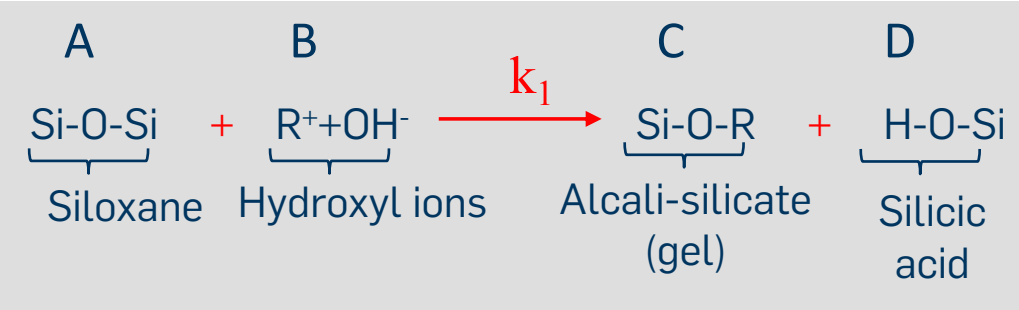
Modell könnte den Unterschied zwischen Schädigungsprozessen in Betonen mit verschiedenen Arten von Gesteinskörnern erklären

Iskhakov, T., Timothy, J.J., Meschke, G. "Expansion and deterioration of concrete due to ASR: micromechanical modeling and analysis" - wurde

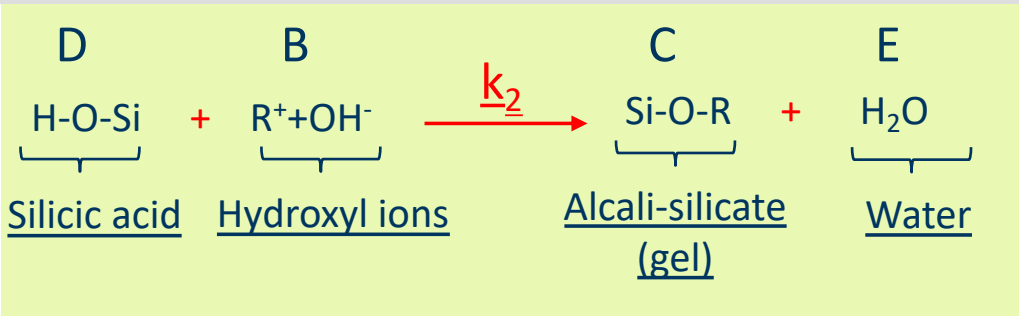
ASR expansion of concrete: Chemical Kinetics

Reaktionsprozesse

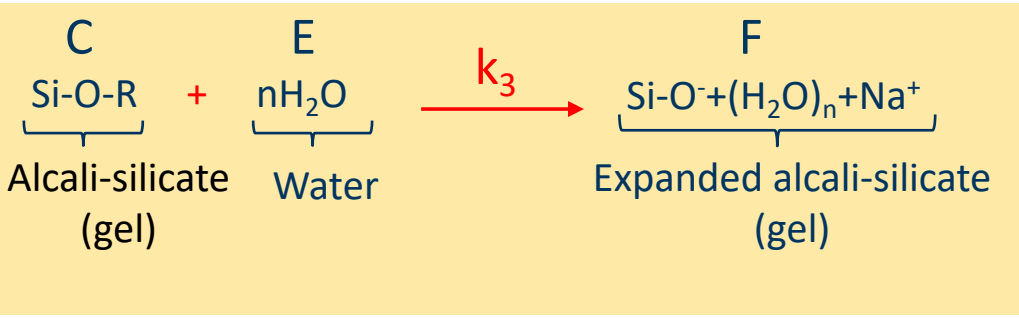
Schritt 1



Schritt 2



Schritt 3



Mathematische Beschreibung

$$\frac{\partial A}{\partial t} = -k_1 A(t)B(t)$$

$$\frac{\partial B}{\partial t} = -k_1 A(t)B(t) - k_2 D(t)B(t)$$

$$\frac{\partial C}{\partial t} = k_1 A(t)B(t) + k_2 D(t)B(t) - k_3 C(t)E(t)$$

$$\frac{\partial D}{\partial t} = k_1 D(t)B(t) - k_2 D(t)B(t)$$

$$\frac{\partial E}{\partial t} = k_2 D(t)B(t) - k_3 C(t)E(t)$$

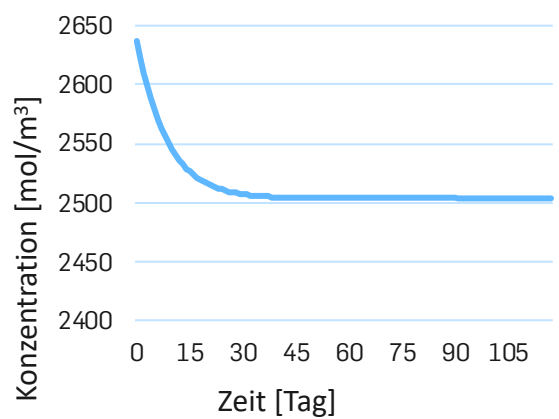
$$\frac{\partial F}{\partial t} = k_3 C(t)E(t)$$

Geschwindigkeitskonstanten $k_1:k_2:k_3 \approx 1:30:60$ (Saouma et al., 2015) basierend auf Dauer der Reaktionen

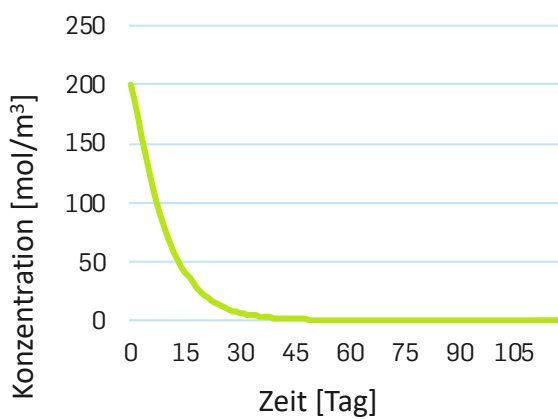
ASR expansion of concrete: Chemical Kinetics

Reaction kinetics leading to formation of expansive ASR gel

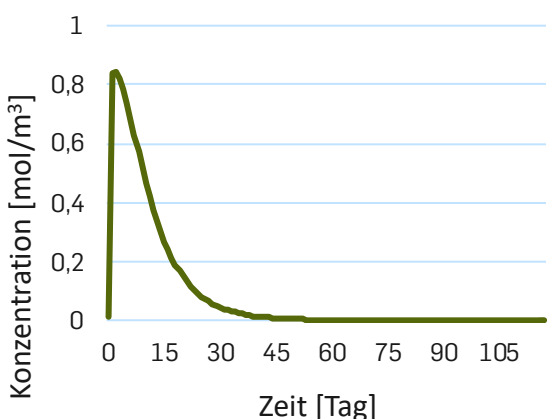
Siloxane



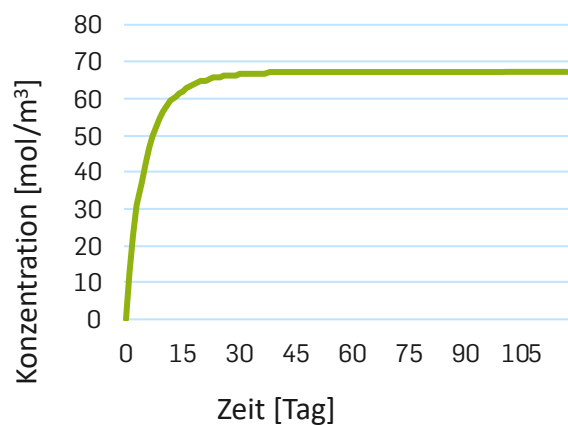
Alkali



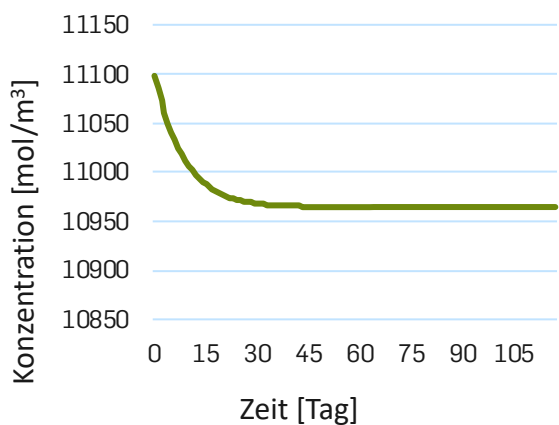
Intermediate reaction product



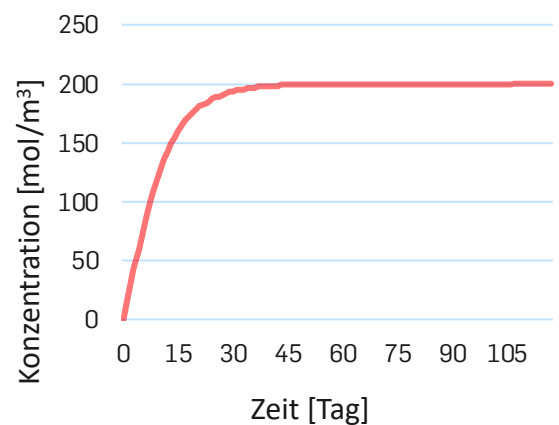
Silicic acid



Water



Expansive alkali silicate gel



Reaktionsmodell

Reaktionsdiffusions-
gleichungen



Zeitabhängige
Konzentration des
Gels $C_{\text{Gel}}(t)$



Zeitabhängiges Volumen
des Gels $V_{\text{Gel}}(t)$ im Korn*
und Zementstein**

Mikromechanisches Modell

Wenn $V_{\text{Gel}}(t) < \text{Volumen der Mikrorisse}$:



Kein Risswachstum

Wenn $V_{\text{Gel}}(t) > \text{Volumen der Mikrorisse}$:



Risswachstum

Makro-Expansion des Betons

Expansion →

Initiation



Entwicklung

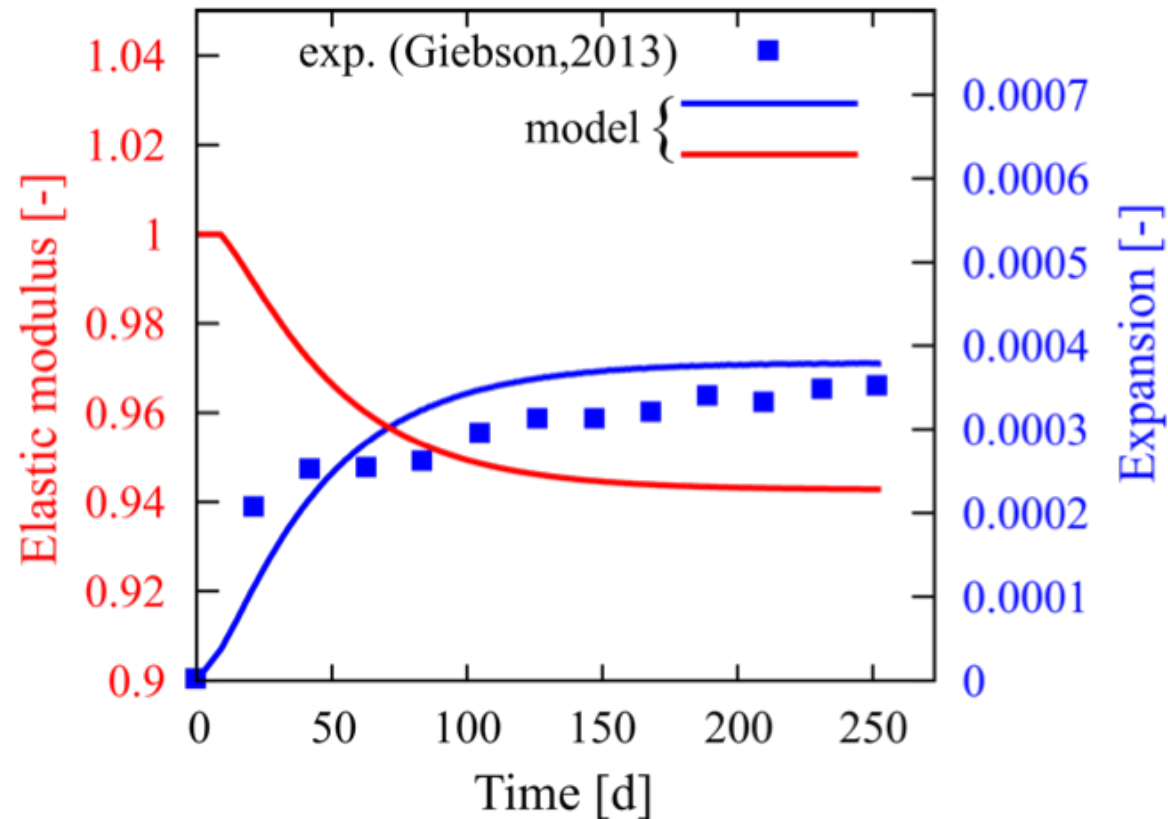


Rest

Zeit ↓

ASR expansion of concrete: Coupling kinetics + Mechanics

Macroscopic expansion due to ASR: Comparison with experimental data



Connectivity of defect distribution must be considered -> Expansive gel does not fill all initial defects in concrete

- Durability of concrete: Multiphysics models supported by multiscale models
- Multiscale models provide input for macroscopic models
 - Macroscopic stiffness, diffusivity & permeability for given pore structure, and state of damage
 - Cascade Continuum Micromechanics (CCM) Model able to predict percolation threshold
 - Dramatic difference of effective permeability below and beyond threshold -determines the effect of damage on transport of aggressive substances
- Example for durability model: Alkali Silica Reaction
 - Phenomenological model: calibration needs specific tests for specific aggregate and concrete composition
 - Multiscale model: attempt to replicate physico-chemical processes of ASR gel production, expansion and deterioration on meso (aggregate) scale
 - Consequence of aggregate type and concrete composition predicted!
 - Upscaling by means of micromechanics methods – macroscopic expansion strains and damage

Research presented was supported by the
German Science Foundation



FOR 1498
ALKALI-SILICA REACTION
IN CONCRETE STRUCTURES

