Teilprojekt 3:
Numerisches Modell zur Beschreibung von Alkalientransport und AKR-induzierter Schädigung in Betonbauteilen

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Multiscale picture of ASR

<table>
<thead>
<tr>
<th>Macroscale [m]</th>
<th>Meso – Microscale [mm - µm]</th>
<th>Nanoscale [nm]</th>
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<tbody>
<tr>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
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</tbody>
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Service life prediction, analysis of effect of cyclic load

Deterioration processes

Ion, water transport

Multifield Finite Element Model

ASR-expansion profile

Multiscale picture of ASR

Pre-existing damage

Pore structure

Alkali-> pore fluid

TP 3: Meschke

Numerisches Modell zur Beschreibung von Alkalientransport und AKR-induzierter Schädigung in Betonbauteilen

20. IBAUSIL 2018
Weimar 12-14 September
Multiscale model for ASR-induced damage

Microcrack

$V_g < V_g^{cr}$

$P_g = 0$

$\dot{P}_g > 0$

REV\textsubscript{Aggregate}

REV\textsubscript{Concrete}

Concrete sample

Kinetics model – formation of ASR-gel

Filling time

Gel pressure

LEFM at microscale

Microporomechanics

Mechanics of ASR

Multifield FE-Model

Macro-Expansion

Initiation

Development

Rest

Laboratory experiments

20. IBAUSIL 2018

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TP 3: Meschke

Numerisches Modell zur Beschreibung von Alkalientransport und AKR-induzierter Schädigung in Betonbauteilen
Modelling damage and expansion of ASR-affected concrete

- Micromechanics based modelling
- Mean-field homogenization

**Concrete REV**
- Concrete = cement paste + embedded spherical aggregates
- Damage localization in cement matrix = annular crack due to aggregate expansion

**Aggregate/cement paste REV**
- Penny-shaped microcracks in aggregate and cement represent pore space
- Microcrack density = const, i.e. no new microcracks are formed
- Microcracks are aligned along 3 orthogonal directions

**Microcrack**
Microcracks = penny-shape: \( X = \frac{c}{a} \ll 1 \)
Upscaling of microcracking processes

Macroscopic expansion and damage

\[ C_{\text{macro}}^{\text{hom}}, E_{\text{macro}} \]

Annular crack initiation and propagation

\[ \sigma_{\theta\theta} = f(E_{\text{agg}}, C_{\text{agg}}^{\text{hom}}, C_{\text{cem}}^{\text{hom}}) \]
\[ K_I(\sigma_{\theta\theta}) - K_{IC} \leq 0 \]

Aggregate expansion due to microcracking

\[ \Sigma = C^{\text{hom}} : E - Bp \]

zero in case of free expansion

gel pressure causing microcrack growth

Growth of penny shaped microcracks in aggregates

\[ \frac{\partial \psi}{\partial \varepsilon} + G_c \geq 0 \]

\( \psi \): potential energy density
\( \varepsilon \): crack density variable

Dormieux, Ulm & Kondo, Wiley, 2006
Comparison with experimental data (TP5 Giebson, 2013)

Elastic modulus vs. macroscopic expansion

The model allows to capture the difference between the damage processes in concrete with different types of ASR-reactive aggregate

Iskhakov, T., Timothy, J.J., Meschke, G. “Expansion and deterioration of concrete due to ASR: micromechanical modeling and analysis” – CCR/in print
Multiscale model for ASR-induced damage

Microcrack in aggregate

\[ V_g < V_g^{cr} \]
\[ P_g = 0 \]
\[ \dot{P}_g > 0 \]

Kinetics of ASR

REV_{Aggregate}  
REV_{Concrete}

Concrete sample

Macro-Expansion
Initiation  
Development  
Rest

LEFM at microscale
Microporomechanics

Expansion

Filling time
Gel pressure

Multifield FE-Model
Kinetics of ASR: reaction mechanism

### Chemical description of ASR

\[
\text{SiO}_2 + 2R^+ + 2\text{OH}^- \rightarrow \text{H}_2\text{SiO}_4^{2-} + 2R^+
\]

\[
\text{H}_2\text{SiO}_4^{2-} + 2R^+ + (\text{Ca}^{2+} + 2\text{OH}^-) \rightarrow \text{CaR}_2\text{SiO}_6\text{H}_4
\]

\[
\text{CaR}_2\text{SiO}_6\text{H}_4 + n\text{H}_2\text{O} \rightarrow \text{CaR}_2\text{SiO}_6\text{H}_4 \cdot n\text{H}_2\text{O}
\]

\[
\text{CaR}_2\text{SiO}_6\text{H}_4 \cdot n\text{H}_2\text{O} + (\text{Ca}^{2+} + 2\text{OH}^-) \rightarrow \text{C-S-H} + 2R^+ + 2\text{OH}^- + n\text{H}_2\text{O}
\]

### Mathematical description

\[
\frac{\partial c^\alpha}{\partial t} = q^\alpha
\]

- \(c\) – concentration
- \(q\) – rate of production/consumption
- \(\alpha\) – \(\text{SiO}_2\), \(R^+\), \(\text{Ca}^{2+}\), \(\text{CaR}_2\text{SiO}_6\text{H}_4\)
- \(k_1, k_2\) – reaction rate coefficients

\[
\frac{\partial c^{\text{SiO}_2}}{\partial t} = -k_1 c^{\text{SiO}_2} c^{R^+}
\]

**Experiment (TP5)**

**BUT:** Employment of experimentally measured (TP5) reaction rate constants reveals that reaction stops almost immediately!

Alkali diffusion into the aggregate is the governing process.
Kinetics of ASR: Slowly Reactive Aggregates

Model: time scale determined by alkali diffusion process into aggregates

\[ c_{Na^+}(x, t) \]

\[ q_{Na^+}(t) \]
Flux due to external alkali supply

Distance to dissolution/reaction site

Measurement of penetrated alkali concentration and expansion in different depths on concrete specimens with and without external alkali supply

Coupling: kinetics + mechanics

If \( V_{Gel}(t) < \) volume of microcracks:

Microcracks don’t grow

If \( V_{Gel}(t) > \) volume of microcracks:

Microcracks grow

Experimental setup (TP5)

\[ c_{Na^+} = \frac{c_0}{x} - \frac{q_{Na^+}(t)}{x} \]

\[ c_0 \]
Initial concentration

\[ x \]
Distance

\[ q_{Na^+}(t) \]
Flux due to external alkali supply

\[ c_{Na^+}(x, t) \]
Alkali concentration at position \( x \) and time \( t \)

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**Kinetics of ASR: Validation**

Model: time scale determined by alkali diffusion process into aggregates

\[
c(x,t) = c_{Na^+}(x,t)
\]

**Flux due to external alkali supply**

\[
q_{Na^+}(t)
\]

**Distance to dissolution/reaction site**

**Measurement of penetrated alkali concentration and expansion in different depths on concrete specimens with and without external alkali supply**

**Model**

- without external \(Na^+\) supply
- 2 cm (with ext. \(Na^+\))
- 4 cm (with ext. \(Na^+\))

**Experiment (TP5)**

- without external \(Na^+\) supply
- 2 cm (with ext. \(Na^+\))
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**Coupling: kinetics + mechanics**

- If \(V_{Gel}(t) < \text{volume of microcracks}\): Microcracks **don’t grow**
- If \(V_{Gel}(t) > \text{volume of microcracks}\): Microcracks **grow**
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- 4 cm (with ext. Na\(^+\))
Application: Expansion and Damage in pavement

Moisture profile
(modelled in partially saturated concrete using Richard’s equation)

Alkali profile
(advective ion transport modelled with upwind scheme)


ASR-gel profile

ASR-expansion profile

ASR-damage profile
Conclusions

• Modelling strategy for ASR-affected concrete behavior:
  • Expansion of aggregate / cement matrix due to growth of ASR-gel filled microcracks
  • Subsequent crack localization in cement matrix caused by aggregate expansion
  • Upscaling by means of micromechanics methods – macroscopic expansion strains and damage
  • Kinetics of ASR is governed by diffusion of alkali ions into aggregate