Validation of Multiscale Model for Heat Generation in Hardening Concrete

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Outline

- Concrete - the second most widely used material
- To yield 2.5 tons per capita per year
- The main raw material cement - participates in 7% carbon dioxide production
Temperature-induced deterioration of concrete structures

- **Mechanical background**
  - Temperature creates strains, which may produce tensile stresses when restraints are present. Low concrete tensile strength may lead to crack formation.

- **Chemical background**
  - Temperature above 70°C causes delayed ettringite formation (DEF). The reaction produces high expansive strains
    \[
    3\text{CaO} \cdot \text{Al}_2\text{O}_3 + 3\text{CaSO}_4 + 26\text{H}_2\text{O} \rightarrow 3\text{CaO} \cdot \text{Al}_2\text{O}_3 \cdot 3\text{CaSO}_4 \cdot 32 \text{H}_2\text{O}
    \]
  - The expansion leads to gaps around aggregates and disintegrates concrete

Gaps around aggregates in field concrete. Railroad sleeper. Fluorescent light. *Courtesy of Concrete Experts International*


Multiscale nature and simulation of concrete

Downscaling
Data acquisition

Hydration models

Sand
Aggregates

C-S-H
Cement paste
Mortar
Concrete
Structure

globules

\[ \text{100 nm} \quad \text{10 \text{ \mu}m} \quad \text{500 \text{ \mu}m} \quad \text{10 mm} \quad \text{10 m} \]

Upscaling
Data compression
CEMHYD3D - model of cement hydration

- Discrete model – voxel (1 x 1 x 1 μm, not much refinement possible)
- 20 year development at NIST, USA

Initial stage  
Hydration  
Fully hydrated

<table>
<thead>
<tr>
<th>C-S-H</th>
<th>Cement paste</th>
<th>Mortar</th>
<th>Concrete</th>
<th>Structure</th>
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<tbody>
<tr>
<td>$10^{-9}$</td>
<td>$10^{-6}$</td>
<td>$10^{-4}$</td>
<td>$10^{-2}$</td>
<td>$10^{-1}$ [m]</td>
</tr>
</tbody>
</table>
Reaction enthalpies

Silicate phases

\[ C_3S(1) + 5.3H(1.34) \rightarrow C_{1.7}SH_4(1.52) + 1.3CH(0.61) \quad [\text{-9\%}], 20^\circ C \quad -517 \text{ J/g} \]

\[ C_2S(1) + 4.3H(1.49) \rightarrow C_{1.7}SH_4(2.07) + 0.3CH(0.191) \quad [\text{-9\%}], 20^\circ C \quad -262 \text{ J/g} \]

\[ 1.1CH(1.34) + S(1) + 2.1H(0.63) \rightarrow C_{1.1}SH_{2.1}(3.0) \quad [+1\%] \quad -780 \text{ J/g}_S \]

Aluminate phases

\[ C_3A(1) + 6H(1.21) \rightarrow C_3AH_6(1.69) \quad [\text{-24\%}] \quad -908 \text{ J/g} \]

\[ C_3A(0.4) + 3C\tilde{S}H_2(1) + 26H(2.1) \rightarrow C_6A\tilde{S}_3H_{32}(3.3) \quad [\text{-6\%}] \quad -1672 \text{ J/g} \]

\[ 2C_3A(0.2424) + C_6A\tilde{S}_3H_{32}(1) + 4H(0.098) \rightarrow 3C_4A\tilde{S}H_{12}(1.278) \quad [\text{-5\%}] \quad -1144 \text{ J/g} \]

\[ C_4AF + 3C\tilde{S}H_2 + 30H \rightarrow C_6A\tilde{S}_3H_{32} + CH + FH_3 \quad [\text{-6\%}] \quad -725 \text{ J/g} \]

\[ 0.575 \quad 1 \quad 2.426 \quad 3.3 \quad 0.15 \quad 0.31 \]

\[ 2C_4AF + C_6A\tilde{S}_3H_{32} + 12H \rightarrow 3C_4A\tilde{S}H_{12} + 2CH + 2FH_3 \quad [\text{-5\%}] \]

\[ 0.348 \quad 1 \quad 0.294 \quad 1.278 \quad 0.09 \quad 0.19 \]

\[ C_4AF + 10H \rightarrow C_3AH_6 + CH + FH_3 \quad [\text{-18\%}] \quad -418 \text{ J/g} \]

\[ 1 \quad 1.41 \quad 1.17 \quad 0.26 \quad 0.545 \]
## Validated experiments - input parameter for CEMHYD3D model

<table>
<thead>
<tr>
<th>Acronym, refer.</th>
<th>C₃Sᵅ</th>
<th>C₂Sᵅ</th>
<th>C₃Aᵅ</th>
<th>C₄AFᵅ</th>
<th>Gypsumᵇ</th>
<th>Fineness [m²/kg]</th>
<th>W/c [-]</th>
<th>Temp. [°C]</th>
<th>$E_a$ [kJ/mol]</th>
<th>$Q_{pot}$ [J/g₉cem.]</th>
<th>$t_0$ [h]</th>
<th>$β$ [h/cycle²]</th>
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<tr>
<td>Aalborg&lt;sup&gt;w,CTU&lt;/sup&gt;</td>
<td>66.60&lt;sup&gt;c&lt;/sup&gt;</td>
<td>23.80&lt;sup&gt;c&lt;/sup&gt;</td>
<td>3.40&lt;sup&gt;c&lt;/sup&gt;</td>
<td>0.40&lt;sup&gt;c&lt;/sup&gt;</td>
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<td>390</td>
<td>0.40</td>
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<td>11.31&lt;sup&gt;de&lt;/sup&gt;</td>
<td>6.16&lt;sup&gt;de&lt;/sup&gt;</td>
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<td>6.64&lt;sup&gt;df&lt;/sup&gt;</td>
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<td>25.0</td>
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<td>40.0</td>
<td>520.38</td>
<td>2.0</td>
<td>3.0E-4</td>
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</table>

<sup>a</sup> Four clinker minerals are later normalized in the CEMHYD3D input routine
<sup>b</sup> Clinker volume is replaced by gypsum or anhydrate in the specified volume fraction
<sup>c</sup> Mineral composition determined directly from XRD / Rietveld analysis
<sup>d</sup> Tested at Czech Technical University in Prague (CTU)
<sup>e</sup> Based on Taylor calculation
<sup>f</sup> Assumed no free lime
<sup>g</sup> Assumed 1.5 wt. % of free lime
<sup>h</sup> Specified in the reference based on Bogue’s calculation
<sup>i</sup> Based on original Bogue calculation
<sup>j</sup> Given 1.5 wt. % free lime, anhydrate 2.94 vol. % and gypsum 3.31 vol. %
<sup>k</sup> Best fit to the measured PSD
<sup>l</sup> Assumed 1.0 wt. % of free lime
<sup>m</sup> Saturated curing conditions
<sup>n</sup> White cement
<sup>o</sup> Estimated
<sup>p</sup> Irrelevant

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**Extra dormant period**

The only degree of freedom of CEMHYD3D model!
Validation of released heat

- Isothermal calorimetry, cement paste

![Graphs of released heat for different w/c ratios and materials](image-url)
Multiscale elastic homogenization

- Upscaling of elasticity from four scales to a concrete material point
- Effect of w/c, fineness, ITZ, aggregates, entrained / entrapped air

Multiscale prediction of elasticity

<table>
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<tr>
<th>Component</th>
<th>Wcr</th>
<th>Density [g/cm³]</th>
<th>Weight [kg/m³]</th>
<th>Volume [dm³]</th>
<th>Weight [kg/m³]</th>
<th>Volume [dm³]</th>
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<td>3.15</td>
<td>370</td>
<td>117.4</td>
<td>550</td>
<td>174.6</td>
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<td>1.0</td>
<td>185</td>
<td>185</td>
<td>148</td>
<td>148</td>
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<td>Plasticizer</td>
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<td>0</td>
<td>3.55</td>
<td>3.55</td>
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<td>Air</td>
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<td>-</td>
<td>0</td>
<td>30.1</td>
<td>0</td>
<td>26.5</td>
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<td>Fine aggregates</td>
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<td>2.51</td>
<td>754</td>
<td>300.4</td>
<td>617</td>
<td>245.8</td>
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<td>Coarse aggregates</td>
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<td>2.64</td>
<td>969</td>
<td>367.05</td>
<td>1060</td>
<td>401.5</td>
</tr>
</tbody>
</table>

**Graphs:**

- **Graph 1:** Young's modulus, E [GPa] vs. Time [days]
  - **Concrete**
  - **Mortar**
  - **Paste**
  - **Paste + air**
  - **Experiment**

- **Graph 2:** Young's modulus, E [GPa] vs. Time [days]
  - **Concrete**
  - **Mortar**
  - **Paste**
  - **Paste + air**
  - **Experiment**

**Legend:**

- **C-S-H**
- **Cement paste**
- **Mortar**
- **Concrete**
- **Structure**
Multiscale simulation of hydration heat

- Transient heat-balance

\[
\nabla^2 T(\mathbf{x}) + \dot{Q}(\mathbf{x}, t) = \rho(\mathbf{x}) \phi_v(\mathbf{x}) \frac{\partial T(\mathbf{x}, t)}{\partial t} \\
\left( \tau K + \frac{1}{\Delta t} C \right) \mathbf{r}^{i+1} = f\left( \mathbf{r}^i, \mathbf{R}^i, \mathbf{R}^{i+1}, \tau, \Delta t \right) \\
K = \int \mathbf{B}^T \mathbf{B} d\Omega \\
C = \int \mathbf{N}^T \rho \phi_v \mathbf{N} d\Omega
\]

![Diagram showing cement paste level and structural level](image.png)

- Heat conduction, FEM

![Graph showing temperature vs. hydration time](image.png)

- C-S-H: $10^{-9}$
- Cement paste: $10^{-6}$
- Mortar: $10^{-4}$
- Concrete: $10^{-2}$
- Structure: $10^{-1}$
Temperature distribution in a railway bridge in Prague

- Prestressed scaffold bridge (12 spans, total length 443 m)
- Known composition of concrete

A new bridge Oparno on the Prague – Dresden highway

- Construction of the bridge (2008-2010)
- Arch span 135 m
- Arches cast in situ from 6m segments
- Budget ~20 mil. €

Progress in 08/2010
Progress in 03/2009
Optimal position of cooling pipes

- Arch casting continues through the whole year – varying temperature
- Massive cast arch segments could attain temperature over 90°C during summer, which is unacceptable
- 12 cooling pipes inserted in the arch
- Two criteria
  - Temperature below 70°C (possible delayed ettringite formation)
  - Reasonable stress field and temperature gradients
Progress in 07/2009
Progress in 08/2010
Ready-mix concrete composition

- **Cement** CEM I 42.5R Prachovice
  - CaO 63.2, SiO₂ 20.8, Al₂O₃ 5.8, Fe₂O₃ 3.3, MgO 3.6, K₂O+Na₂O 2.1, free CaO 0.88, SO₃ 2.85
  - Bogue: C₃S 43.76, C₂S 26.63, C₃A 9.79, C₄AF 10.04
  - Blaine fineness 320 m³/kg

- **Concrete** C45/55 XF2
  - Cement 431 kg/m³ in which 5% SCM
  - Water 178 kg/m³, w/b = 0.413
  - Aggregates 1785 kg/m³
  - Superplasticizer 4.19 kg/m³
  - Silica fume 30 kg/m³
  - Limestone 30 kg/m³
  - Entrained/entrapped air 2.8 %
Multiscale modeling approach

- Coupled cement hydration model on microscale with FEM on macroscale
- Eight cement microstructures 50x50x50 μm assigned to color regions
- Simulation runs ~30 minutes covering several weeks after casting
Multiscale simulation with coupled mechanics

1. No cooling
2. Original cooling
3. Optimized cooling
4. Stress distribution
Effect of pipe cooling in summer

- Ambient air temperature 30°C
Validation – simulation with real conditions

- Measured temperature in the 4th segment, in the centroid
1. Mass concrete & cement hydration models

**Definition:** ▪ concrete exceeding ~0.5 m in the smallest dimension

**Concrete:** ▪ low thermal conductivity
  ▪ exothermic hydration process
  ▪ internal temperature gradients

**Problems:** ▪ tensile stresses = age cracking
  ▪ compromise concrete durability

**Prevention:** ▪ maximum differential temperature is limited to 20°C
  ▪ temperature in concrete should not exceed 70°C

**Prediction:** ▪ Hydration model: CEMHYD3D and Thermo-Chemo-Mechanical
1. Mass concrete & cement hydration models

**CEMHYD3D:** cellular automata approach to simulate microstructural evolution of hydrating cement paste

**TCM-model:** the hydration is modeled based on the theory of reactive porous media (diffusion of free water through layers of hydration products)

**Drawback:** they demand a large number of parameters. Several of these have to be obtained based on adiabatic/isothermal experiments.

**Trends:** hydration models with few input parameters

**Problems with adiabatic or isothermal measurements:**
2. Objectives

- Propose a semi-adiabatic experimental setup – *Temperature measurements*

- Calibrate a hydration model based on experimental results – *Calibration*

- Predict the thermal behavior of a mass concrete structure – *Validation*

*Figure 1: Multiscale model for heat generation in hardening concrete*
3. Heat transport & affinity hydration model

**Affinity hydration model** (Chemical affinity of the reactants)

Parametric function: $\beta_1$, $\beta_2$, $\eta$, and $\text{DoH}_\infty$

$$\tilde{A}_T = \tilde{A}_{25,\exp} \left[ \frac{E_a}{R} \left( \frac{1}{273.15 + 25} - \frac{1}{T} \right) \right]$$

$$\frac{d\text{DoH}}{dt} = \tilde{A}_{25}(\text{DoH}) = B_1 \left( \frac{B_2}{\text{DoH}_\infty} + \text{DoH} \right) (\text{DoH}_\infty - \text{DoH}) \exp \left( -\eta \frac{\text{DoH}}{\text{DoH}_\infty} \right),$$

**Heat transport**

$$C\dot{\mathbf{r}} + K\mathbf{r} = \mathbf{p},$$

$$K = \int_{\Omega} \mathbf{B}(\mathbf{x})^T \lambda(\mathbf{x}) \mathbf{B}(\mathbf{x}) d\Omega, \quad [\text{Conductivity}]$$

$$C = \int_{\Omega} \mathbf{N}(\mathbf{x})^T \rho(\mathbf{x}) c_V(\mathbf{x}) \mathbf{N}(\mathbf{x}) d\Omega, \quad [\text{Heat capacity}]$$

$$\mathbf{p} = -\int_{\Gamma_{c,T,q}} \mathbf{N}(\mathbf{x})^T \mathbf{n}(\mathbf{x})^T q(\mathbf{x}, t) d\Gamma + \int_{\Omega} \mathbf{N}(\mathbf{x})^T \mathbf{Q}(\mathbf{x}, t) d\Omega, \quad [\text{Heat load vector}]$$
4. Semi-adiabatic experimental setup

- Fresh concrete is placed into the semi-adiabatic setup
- The temperature evolution is measured by Type-K thermocouples
  - The measurements are collected by a datalogger
5. Calibration of the affinity hydration model

Concrete composition:

<table>
<thead>
<tr>
<th>Materials</th>
<th>CI</th>
</tr>
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<tbody>
<tr>
<td>Cement CP IV RS(^{(1)})</td>
<td>420</td>
</tr>
<tr>
<td>River Sand (S)</td>
<td>750</td>
</tr>
<tr>
<td>Coarse Aggregate 1 (Max. grain size: 12.5 mm)</td>
<td>1020</td>
</tr>
<tr>
<td>Coarse Aggregate 2 (Max. grain size: 25.0 mm)</td>
<td></td>
</tr>
<tr>
<td>Water</td>
<td>138.6</td>
</tr>
<tr>
<td>Crushed ice</td>
<td>59.4</td>
</tr>
<tr>
<td>Water reducing admixture(^{(2)})</td>
<td>0.65%</td>
</tr>
<tr>
<td>High range water reducing admixture(^{(2)})</td>
<td>0.44%</td>
</tr>
</tbody>
</table>

Thermal properties of concrete:

- Thermal Conductivity = \(1.8 \text{ Wm}^{-1}\text{K}^{-1}\)
- Heat capacity = \(870 \text{ Jkg}^{-1}\text{K}^{-1}\)
- \(Q_{pot}\) of cement = \(518.37 \text{ J/g}\)

Parameters: \(\beta_1 = 0.0007 \text{ s}^{-1}\), \(\beta_2 = 6.0e\text{-}5\), \(\eta = 6.1\), \(\text{DoH}_\infty = 0.85\), and \(E_a = 38.3 \text{ kJ/mol}\).

\(T_{\text{max}} = 55.2 \, ^{\circ}\text{C} / t = 16\text{h}\)
6. Case study

Mass concrete foundation block:

- Concrete composition C1
- Size - 19.60 x 10.10 x 2.50 m

- Two layers of concrete – 12h casting
- Curing method - ponding water
- 6 gauges were placed in the block

OOFEM model: (1/4 - Block Symmetry)

- 3840 brick elements / 4641 nodes
- Integration step = 2h, Total 100 steps

- Soil density = 2000 kg/m³
- Thermal conductivity = 0.8 Wm⁻¹K⁻¹
- Heat capacity = 840 Jkg⁻¹K⁻¹

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6. Case study (Validation)

**OOFEM model:**

- Good agreement between results (2,4,6)
- Minor influence of boundary conditions (1,5)
- The results validated the multiscale model

**Simulation vs. Experimental results**

\[ T_{\text{max}} = 65.0 \, ^\circ C / t = 74h \]
The proposed setup is a suitable alternative to isothermal calorimeter.

The proposed setup is attractive for the concrete industry due to its low cost.

The affinity hydration model can be applicable to any shape and size.

The upscaling of laboratory experiments enables time-efficient simulation.

Figure 1: Multiscale model for heat generation in hardening concrete
Conclusions

- Multiscale modeling can be incorporated to a majority of codes
- The implementation into code for HOLCIM was finished this year
- Multiscale models have several parameters which need to be identified, but promise high accuracy
- Presented multiscale model implemented in an open-source, object oriented finite element package, see [http://www.oofem.org](http://www.oofem.org)
- Simplified version was developer for IPHONE
- Optimization of cooling pipes significantly reduced crack induction and extends lifetime of the arches and bridge
- New contract with Holcim
Thank you for your attention!

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