Research project „Innovative cement based materials and concrete with high calcium fly ashes”
co-financed by the European Union from the European Regional Development Fund

Michal A. Glinicki

Determination of Thermal Properties of Unconventional Concrete During Hardening

Institute of Fundamental Technological Research
Polish Academy of Sciences
Warsaw, Poland

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Outline of presentation

1. Introduction/motivation
2. Objectives of investigation
3. Model formulation and IHTP solution (TMC software)
4. Experimental data input (1D)
5. Verification in 2D
6. Predicted and measured temperature in large blocks
7. Conclusions
CO₂ emission in cement industry in Poland

- Average emission from 251 European cement plants: **868 kg CO₂/ton clinker**, average biomass content in fuel 6.7%
- Actual emission in cement industry in Poland: **823 kg CO₂/ton clinker**
- Empirical benchmark (Directive 2003/87/EC) from 10% of the best low emission cement plants in Europe: **766 kg CO₂/ton clinker** (biomass factor >25%)

**Advantages:** low electricity consumption; high fuel substitution (45%); high clinker substitution (CF = 0.77 )

**Threat =** European Union Emissions Trading System (EU ETS) → lack of about 4.5 million ton of CO₂ allowances annually
Clinker production at risk in Poland due to high price of carbon emissions in EU ETS

~100% of clinker production at risk with a CO₂ price of €23/t 0% free allowances allocated

<table>
<thead>
<tr>
<th>CO₂ prices (€/t)</th>
<th>Distance (km) from border to isolate</th>
<th>% of total clinker production at risk</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>150</td>
<td>15</td>
</tr>
<tr>
<td>13</td>
<td>250</td>
<td>23</td>
</tr>
<tr>
<td>16</td>
<td>350</td>
<td>54</td>
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<tr>
<td>20</td>
<td>450</td>
<td>77</td>
</tr>
<tr>
<td>23</td>
<td>550</td>
<td>100</td>
</tr>
</tbody>
</table>

Isolines of production at risk for different CO₂ prices based on inland transportation costs in Poland from Ukraine.

1. For clinker from Ukraine
Note: Clinker production by plant estimated as average being a confidential information; Distance from the plant in Ukraine to main entrances is 50 km
Source: Cembureau; Polish Cement Association
The thermal properties of concrete, whether the concrete is massive or in thin sections, are the properties that are most ignored and the least understood by the general concrete engineering and construction industry…

Stephen B. Tatro

OBJECTIVES OF INVESTIGATION

- to develop numerical tools for determination of transient temperature field in concrete during hardening
- to establish the range of possible applications of concrete containing new blended cements
Heat transfer equation to describe the transient temperature field in hardening concrete

\[ c\rho \frac{\partial T}{\partial t} - \frac{\partial}{\partial x} \left( k_x \frac{\partial T}{\partial x} \right) - \frac{\partial}{\partial y} \left( k_y \frac{\partial T}{\partial y} \right) - \frac{\partial}{\partial z} \left( k_z \frac{\partial T}{\partial z} \right) = Q \]

where: \( T \) – temperature, \( t \) – time, 
\( x, y, z \) space coordinates, 
\( \rho \) – density, \( c \) – heat capacity, 
\( k_x, k_y, k_z \) thermal conductivity in direction \( x, y, z \) respectively. 
\( Q \) - internal heat source

the coefficients are time, space and temperature dependent
Solution of heat transfer equation:

→ direct solution
requires fine identification of material parameters,
fails when less known (unconventional) components are used

→ inverse solution
- one dimensional heat flow equation
- the temperature field is estimated on
  the basis of temperature measurement
  in several points in one dimensional mold
- solution of the optimization problem for
  given initial and boundary conditions
Thermal & Mechanical modelling of Concrete

**TMC software**
Solution of inverse heat transfer problem

functions $k$, $c$ and $Q$ are parameterized:

$$k_x = k_y = k_z = k(t_e) = \begin{cases} a_k t_e + b_k, & 0 \leq t_e < 72h \\ 72a_k + b_k, & t_e \geq 72h \end{cases}$$

$$c = c(t_e) = \begin{cases} a_c t_e + b_c, & 0 \leq t_e < 72h \\ 72a_c + b_c, & t_e \geq 72h \end{cases}$$

$$Q = Q(t, t_e) = \frac{t_e}{t} \sum_{i=1}^{n} q_i N_i(t_e)$$

$t_e$ is the equivalent time:

$$t_e = \int_0^t \beta(T)dt' = \int_0^t \exp\left(\frac{E}{R \left(\frac{1}{293} - \frac{1}{273 + T}\right)}\right)dt'$$

$E$ is the activation energy and $R$ is the universal gas constant

$N_i$ are linear shape functions for a one dimensional finite element

$a_k$, $b_k$, $a_c$, $b_c$, $q_i$ are unknown coefficients to be determined
the calculated temperature $T^n$ is compared with the measured temperature $T^e$ to define the objective function to be minimized:

$$E(a) = (T^e - T^n)^T (T^e - T^n) + \gamma \sum_{p=1}^{P} a^2_p$$

where $\gamma$ is a regularization parameter,
$a_p$ unknown parameters ($a_p=\{a_k, b_k, a_c, b_c, q_i\}$),
$P$ is a number of unknown parameters.

the objective function $E$ is minimized by non-gradient direct search algorithm

to avoid non-uniqueness of solution the IHTP is solved twice
Experimental data input: one dimensional mould

position of temperature sensors
Results of 1D measurements
Results of inverse heat transfer solution in 1D

<table>
<thead>
<tr>
<th>c(t_e)</th>
<th>b_c [J/kgK]</th>
<th>Mixture</th>
</tr>
</thead>
<tbody>
<tr>
<td>c(t_e)</td>
<td>b_c [J/kgK]</td>
<td>Mixture</td>
</tr>
<tr>
<td>PP-50-0</td>
<td>0.0578 915.77</td>
<td>PP-50-0</td>
</tr>
<tr>
<td>P-50-00.0</td>
<td>0.1928 910.1</td>
<td>P-50-0</td>
</tr>
<tr>
<td>P-50-60 WS</td>
<td>0.0729 912.1</td>
<td>P-50-60 WS</td>
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<table>
<thead>
<tr>
<th>k(t_e)</th>
<th>b_k [W/mK]</th>
<th>Mixture</th>
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<tbody>
<tr>
<td>a_k [W/mK]</td>
<td>b_k [W/mK]</td>
<td>Mixture</td>
</tr>
<tr>
<td>PP-50-0</td>
<td>-0.0021 1.628</td>
<td>PP-50-0</td>
</tr>
<tr>
<td>P-50-00.0</td>
<td>-0.0037 1.592</td>
<td>P-50-0</td>
</tr>
<tr>
<td>P-50-60 WS</td>
<td>-0.0018 1.398</td>
<td>P-50-60 WS</td>
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</tbody>
</table>
VERIFICATION
2D calculations and measurements

Trapezoidal shape element
Thermally isolated mould (except the upper surface)
Set of temperature sensors positioned in the mould
Predicted and measured temperature in 2D element

position of temperature sensors
Predicted and measured temperature in large concrete blocks

Thermally isolated mould (~0.8 m³)
Set of positioned temperature sensors
Temperature field in concrete block

Equal binder content:
- CEM I portland cement
- CEM II B-S + HCFA

no thermal isolation at 1 side
Effect of cement composition on temperature field in concrete block

### Composition of new blended cements

<table>
<thead>
<tr>
<th>Cement type</th>
<th>Clinke r</th>
<th>HCF A</th>
<th>Fly ash</th>
<th>Slag</th>
<th>Gypsum</th>
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</thead>
<tbody>
<tr>
<td>CEM I</td>
<td>94.5</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>5.5</td>
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<tr>
<td>CEM II/A-W</td>
<td>80.9</td>
<td>14.3</td>
<td>-</td>
<td>-</td>
<td>4.8</td>
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<tr>
<td>CEM II/B-W</td>
<td>67.4</td>
<td>28.9</td>
<td>-</td>
<td>-</td>
<td>3.7</td>
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<tr>
<td>CEM II/B-M (V-W)</td>
<td>66.6</td>
<td>14.3</td>
<td>14.3</td>
<td>-</td>
<td>4.8</td>
</tr>
<tr>
<td>CEM II/B-M (S-W)</td>
<td>66.6</td>
<td>14.3</td>
<td>-</td>
<td>14.3</td>
<td>4.8</td>
</tr>
<tr>
<td>CEM V/A (S-W)</td>
<td>47.9</td>
<td>23.9</td>
<td>-</td>
<td>23.9</td>
<td>4.2</td>
</tr>
</tbody>
</table>

![Graph showing max Δ T °C for different concrete blocks]
CONCLUSIONS

- Thermal properties of hardening concrete were effectively determined using unconventional approach—the inverse heat transfer problem solution using 1D temperature measurements and optimization by non-gradient direct search algorithm.
- Determination of transient temperature field in hardening concrete is possible for unknown mix composition.

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