Modeling of concrete at early age, benchmark carried out within COST TU 1404

WG2 – Modelling of CBMs and the behaviour of structures

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Agnieszka KNOPPIK – Silesian University of Technology, Poland
Laurie LACARRIERE – LMDC, France
Mateusz WYRZYKOWSKI – Empa, Switzerland
1. DESCRIPTION OF THE COST ACTION (www.tu1404.eu)

2. OBJECTIVE & PROGRAM OF THE WG 2
   a) STAGE 1: Simple examples
   b) STAGE 2: RRT+ and durability
   c) STAGE 3: Real structures

CONCLUSION & PERSPECTIVES
What is COST?

COST is the oldest and widest European intergovernmental framework for Cooperation in Science and Technology (1971)

COST Countries

What is a COST Action?

pan-European, bottom-up science and technology networks open to researchers, industry and policy stakeholders

Duration 4 years.
Minimum 5 COST member countries

COST supports the following networking activities:

- Meetings, Conferences, Workshops, Short-term scientific exchanges,
- Training schools, Publications & dissemination activities
COST Action TU1404

Towards the next generation of standards for service life of cement-based materials and structures

The main objective of the Action is to develop a new generation of guidelines/recommendations to predict/evaluate the service life of cement based materials and structures in Europe by integrating the most recent developments in experimental and numerical approaches, with particular focus on concrete performance since early ages.

- Mutual validation and benchmarking
- Development of new products together with industry partners
- Drafting of standardization-targeted documentation
Scientific program of TU1404
Current participation and leadership

286 participants from 31 countries

41% Early Stage Researchers
43% Inclusiveness countries
2/3 Gender balance

Chair: Miguel Azenha (PT)
Vice-Chair: Stéphanie Staquet (BE)
General Secretary: Dirk Schlicke (AT)

WG1 – Testing of Cement-Based Materials (CBM)
Leadership: M. Serdar (HR), S. Nanukuttan (UK), E. Roziere (FR)

WG2 – Modelling of CBMs and the behaviour of structures
Leadership: Agnieszka Knoppik (PL), Mateusz Wyrzykowski (CH)
Farid Benboudjema (FR), Laurie Lacarriere (FR)

WG3 – Development of recommendations and products
Leadership: François Toutlemonde (FR) and Terje Kanstad (NO)
Our website: www.tu1404.eu

JOIN THE ACTION!

http://www.tu1404.eu/join-the-action
1. DESCRIPTION OF THE COST ACTION (www.tu1404.eu)

2. OBJECTIVE & PROGRAM OF THE WG 2
   
a) STAGE 1: Simple examples
   b) STAGE 2: RRT+ and durability
   c) STAGE 3: Real structures

CONCLUSION & PERSPECTIVES
Objectives of WG2

**Objective 1:**
Predict properties of concrete only by knowing its concrete mix design (WG1)

**Objective 2:**
Knowing properties of concrete (prediction/experiment), to perform calculations on real structures (→ cracking) → durability

*Allow for numerical experiments in order to optimize composition regarding requested properties: mechanical, cost, ecological etc.*

**Objective 3:**
Link with design software and recommendations (WG3)
WORKING GROUP 2 DESCRIPTION

Modelling and Benchmarking

GP2.a – Microstructural modelling
Guang Ye, The Netherlands & Smilauer Vit, Czech Republic

GP2.b – Multiscale modelling
Dunant Cyrille, Switzerland & Pichler Bernhard, Austria

GP2.c – Macroscopic modelling
Gawin Dariusz, Poland & Briffaut Matthieu, France

GP2.d – Probabilistic modelling (sensitivity analysis)
Hendriks Max, Norway & Caspeele Robby, Belgium

GP2.e – Durability
Galvez Jaime C., Spain & Ravi Patel, Belgium

GP2.f – Benchmarking calculations
Lacarrière Laurie, France & Knoppik-Wróbel Agnieszka, Poland
BENCHMARK Stage 1

The idea:

to compare different modelling tools used by the participants, to try to settle a guide for verification and validation of computations at early-age.

The examples:

• fully open, i.e. the participants have access to all input data as well as final results;

• based mostly on published experimental data.

The simulations are focused both on material properties and structural phenomena.

MACROSCOPIC & MICROSCOPIC calculations (Not presented today)
Benchmark stage 1: MACRO-modelling

**Example 1:** simple theoretical examples

**Example 2:** experimental example focused on thermal analysis

**Example 3:** experimental example focused on stress analysis

<table>
<thead>
<tr>
<th></th>
<th>DECLARED</th>
<th>CONTRIBUTED</th>
</tr>
</thead>
<tbody>
<tr>
<td>EXAMPLE 1</td>
<td>12</td>
<td>6</td>
</tr>
<tr>
<td>EXAMPLE 2</td>
<td>10</td>
<td>4</td>
</tr>
<tr>
<td>EXAMPLE 3</td>
<td>9</td>
<td>3</td>
</tr>
</tbody>
</table>

2 rounds in order to give more explanations and correct some eventual mistakes
Benchmark stage 1: MACRO-modelling

Participants

Miguel Azenha & Jose Granja University of Minho, Portugal

Farid Benboudjema ENS Paris-Saclay, France

Arnaud Delaplace LafargeHolcim Research Center, France

Dirk Schlicke & Peter Joachim Heinrich Technical University of Graz, Austria

Giuseppe Sciumè University of Bordeaux, France & Stefano Dal Pont Université Grenoble Alpes UGA, France

Vít Šmilauer & Karolína Hájková Czech Technical University in Prague, Czech Republic

Vyacheslav Trojan Kyiv National University of Construction and Architecture, Ukraine

Different softwares, experiences, mesh, models etc.
Benchmark stage 1: MACRO-modelling

**EXAMPLE no. 1**

Modelling of thermo–chemical and mechanical behaviour of basic elements.

**Input:**
- mix composition and conditions of testing,
- adiabatic temperature development for two different initial temperatures,
- thermo–chemical and mechanical properties
- Initial and boundary conditions etc.

**Output:**
- temperature development in time,
- stress development in time (elastic and visco-elastic analysis).

Provided by: F. Benboudjema
farid.benboudjema@ens-cachan.fr
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1

<table>
<thead>
<tr>
<th>Material properties</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Volumetric thermal capacity</td>
<td>2.40E+06 J/m³K</td>
<td></td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>1.75 W/m²K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Initial conditions</th>
<th></th>
<th></th>
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<tbody>
<tr>
<td>T₀</td>
<td>20°C</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Boundary conditions</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>T_air</td>
<td>20°C</td>
<td></td>
</tr>
<tr>
<td>Global coefficient for thermal exchange</td>
<td>10 W/m²K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Geometry</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Width</td>
<td>2 m</td>
<td></td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Concrete composition</th>
<th></th>
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<tbody>
<tr>
<td>Cement</td>
<td>400 kg/m³</td>
<td>Rochefort CEM I 52,5 N CP2 NF (2001)</td>
</tr>
<tr>
<td>Water</td>
<td>180 kg/m³</td>
<td></td>
</tr>
<tr>
<td>Sand (0/4)</td>
<td>730 kg/m³</td>
<td></td>
</tr>
<tr>
<td>Gravel (5/16)</td>
<td>376 kg/m³</td>
<td></td>
</tr>
<tr>
<td>Gravel (12/20)</td>
<td>700 kg/m³</td>
<td></td>
</tr>
<tr>
<td>Admixture</td>
<td>1 kg/m³</td>
<td>Cimplast 115, Axim</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Properties of cement</th>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Compressive strength at 2 days</td>
<td>33 MPa</td>
<td>on normalized mortar</td>
</tr>
<tr>
<td>Compressive strength at 2 days</td>
<td>60 MPa</td>
<td>on normalized mortar</td>
</tr>
<tr>
<td>Heat Release at 41 hours</td>
<td>324 J/g of cement</td>
<td>on normalized mortar</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Content of mineral phases</th>
<th></th>
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<tbody>
<tr>
<td>C₃S</td>
<td>58%</td>
<td></td>
</tr>
<tr>
<td>C₂S</td>
<td>24%</td>
<td></td>
</tr>
<tr>
<td>C₃A</td>
<td>7%</td>
<td></td>
</tr>
<tr>
<td>C₄AF</td>
<td>11%</td>
<td></td>
</tr>
</tbody>
</table>
**Benchmark stage 1: MACRO-modelling**

**EXAMPLE no. 1**

**CASE 1**
- experimentally-determined adiabatic temperature,
- perfectly restrained,
- uniform field of temperature,
- uniform stress (3D),
- Total strain $\varepsilon = 0$.

**CASE 2**
- imposed semi-adiabatic temperature,
- end-restrained,
- uniform field of temperature,
- uniform stress (1D),
- uniform strain.
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1

CASE 3

Thermo-chemical simulations

0.5 m

No flux

Exchange by convection
\( h = 10 \text{ W.m}^{-2}.\text{K}^{-1} \)

Initial temperature: 20°C
Ambient temperature: 20°C

Elastic mechanical simulations

Plane stress conditions: \( \sigma_{xx} = \sigma_{yy} = \sigma_{yz} = 0 \)

Axis of symmetry

1 m

No flux

y

z

x

A

B
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1: Adiabatic temperature

Evolution of temperature in adiabatic test 1

$T_i = 22^\circ C$

Identification of hydration parameters and release of heat

Evolution of temperature in adiabatic test 2

$T_i = 12^\circ C$
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1: Temperature in a wall

Dot A (center of the specimen)

Thermo-chemical simulations (dot A)

Prediction of maximal temperature 😊

2 rounds benchmark was useful
Note that $E_a/R$ is equal to 5080 K and 4510 K for teams 2 and 4!
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1: Temperature in a wall

Dot B (surface of the specimen)

Thermo-chemical simulations (dot B)

Prediction of gradient of temperature 😊

Change of output, team 6 has plot the evolution at a distance of 10 cm
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1: Autogenous shrinkage

1 & 2

Shrinkage proportional to degree of hydration with final value -107 μm/m

3

Elastic and creep under capillary pressure

5

\[ \varepsilon_{\text{cas}}(t) = \varepsilon_{\text{cas,28}} \cdot \exp \left\{ b \cdot \ln \left( 1 + \frac{t}{\tau_k} \right)^a \right\} \]

6

Fib Model Code 2010 with final value -220 μm/m

Better fitting at short term, but not at long term, depending on the model type

→ Comparison may not be relevant!
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1: Modulus of elasticity and creep

2

• **Modulus of elasticity:** after de Schutter law

• **Creep:** Burger model with dependance on hydration degree

6

• **Modulus of elasticity:** B3 model

• **Creep:** B3 model with ageing expressed by equivalent age

\[ E_c(t) = E_{cm} \cdot \left[ \exp \left\{ -a \cdot \frac{w}{z} \cdot (t_{eff}^{\beta_{wes}} - 28^{\beta_{wes}}) \right\} \right]^{-1/3} \]

Fitting is sometimes not possible, depending on the model type

\[ \Rightarrow \text{Comparison may not be relevant!} \]
Benchmark stage 1: MACRO-modelling
EXAMPLE no. 1

**CASE 1**

- experimentally-determined adiabatic temperature,
- perfectly restrained,
- uniform field of temperature,
- uniform stress (3D),
- Total strain $\varepsilon = 0$. 

![Diagram](image)
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1

CASE 1

- experimentally-determined adiabatic temperature,
- perfectly restrained,
- uniform field of temperature,
- uniform stress (3D),
- Total strain $\varepsilon = 0$.

Compressive stresses $\Rightarrow$ 😊
Significant differences, that was not expected since behavior is elastic $\Rightarrow$ ☹️ (especially team 1)

$$\dot{\sigma}_{ii} = - \frac{E(t)}{1-2\nu} \dot{\varepsilon}_{sh}$$

More differences when creep is taken into account (expected)
Benchmark stage 1: MACRO-modelling
EXAMPLE no. 1

CASE 3

Thermo-chemical simulations

0.5 m
No flux

No flux

Exchange by convection
($h = 10 \, \text{W.m}^{-2}.\text{K}^{-1}$)

Initial temperature: 20°C
Ambient temperature: 20°C

Elastic mechanical simulations
Plane stress conditions: $\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = 0$

Temperature prediction was OK ☺️
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 1

Example of stress analysis: boundary conditions 2

Vertical stresses in dot B (MPa) - No creep

Huge differences! Team 1 and 4 are closed now!

More differences when creep is taken into account (expected)

\[
\dot{\varepsilon} = \dot{\varepsilon}_e + \dot{\varepsilon}_{sh}
\]

\[
\dot{\varepsilon}_e = \frac{1 + \nu}{E(t)} \dot{\sigma} - \frac{\nu}{E(t)} tr(\dot{\sigma}) I
\]
DISCUSSION OF EXAMPLE 1

- Temperature predictions are very close

- Some softwares do not allow 2D stress plane conditions, or to impose evolution of internal temperature

- Some models are based on constitutive equations which cannot fit evolutions of material parameters,
  - finite element results are no more comparable in the sense of an educational booklet
  - But it is interesting to quantify errors due to the modelling approach

- No significant differences in elastic calculations should be expected if evolutions of material properties are precisely fitted

- A 3\textsuperscript{rd} round is necessary before publishing
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 2

Modelling of 3D temperature field in a concrete cube.

Input:

• concrete composition,
• geometry of the cube,
• environmental conditions (50% RH, 20°C),
• isothermal calorimetry curves at different temperatures (20, 30, 40, 50, 60°C),
• temperature development in different locations (with sensors) and thermographic images of cube surfaces.

Output:

• temperature distribution in space and development in time.

Provided by: M. Azenha
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Benchmark stage 1: MACRO-modelling

EXAMPLE no. 2: Temperature
Comparison of temperature evolution measured by sensors in different locations in the sample. **Sensor TP3**

![Graph showing temperature evolution over time for Sensor TP3 with different lines representing measured and numerical data.](image)

**Surface sensor**
The effect of formwork removal should be visible.
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 2: Temperature

Comparison of temperature evolution measured by sensors in different locations in the sample. Sensor TP18

Core sensor
Allows to determine maximum temp.
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 2: Temperature
Comparison of identification of material parameters

$Q(t) = Q_{\text{max}} \cdot \exp \left\{ b \cdot \ln \left( 1 + \frac{t_{\text{eff}}}{\tau_k} \right)^a \right\}$

$t_{\text{eff}} = \int \exp \left\{ \frac{A}{8.3143} \cdot \left[ \frac{1}{293} - \frac{1}{273 + T(t)} \right] \right\} \, dt$

Thermo-activation should be taken into account!
Benchmark stage 1: MACRO-modelling

DISCUSSION OF EXAMPLE 2

• Temperature predictions are very close as in example 1, if boundary conditions are taken into account and if isothermal calorimetry experiments are well reproduced
Benchmark stage 1: MACRO-modelling

**EXAMPLE no. 3**

Modelling of temperature and stress development in time of an element in a passive restraining frame.

**Input:**
- concrete mix composition,
- thermo–chemical and mechanical properties,
- geometry of a sample and testing setup,
- adiabatic temperature rise,
- temperature development in the core/in the corner,
- average stress.

**Output:**
- temperature development in time,
- stress development in time (elastic behaviour and with identification of creep).

Provided by: D. Schlicke

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Benchmark stage 1: MACRO-modelling

EXAMPLE no. 3

Restraining frame experiment (at TU Graz)

Set-up:

- Load cell
- Specimen ($l = 3.70$ m)
- 4 x frictionless support

Idealisation:

Specimen is insulated
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 3

Mix composition of concrete used in restraining frame experiment

<table>
<thead>
<tr>
<th>component</th>
<th>amount</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>CEM III/A 32.5N Holcim</td>
<td>300</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Water</td>
<td>145</td>
<td>kg/m³</td>
</tr>
<tr>
<td>Aggregates 0/16</td>
<td>2000</td>
<td>kg/m³</td>
</tr>
<tr>
<td>BV ViscoCrete-1051 PCE</td>
<td>3</td>
<td>kg/m³</td>
</tr>
</tbody>
</table>

+ Thermal properties of concrete used in restraining frame experiment (measured or retrofitted)
+ Mechanical properties of concrete used in restraining frame experiment

![Graph showing temperature development](image1)

![Graph showing average stress development](image2)

Removal of the formwork

Temperature, °C

-20 0 20 30 40 50

Time, h

-1.5 -1.0 -0.5 0.0 0.5 1.0 1.5 2.0 2.5

Average stress, MPa

100 200 300 400
Benchmark stage 1: MACRO-modelling
EXAMPLE no. 3

Simplified boundary conditions (formwork not meshed)

\[ \phi_{\text{conv}} = h(T_s - T_{\text{air-ext}}) \]

\[ h = 0.5 \text{ W}/(\text{m}^2\text{K}) \]

Realistic boundary conditions (formwork meshed)
Benchmark stage 1: MACRO-modelling

EXAMPLE no. 3

Calculation of the mean stress in concrete

Creep is taken into account

Few differences are found (results have been given)

Creep is not taken into account

In this case, it could have been not safe

Tensile stresses occur later (depending on the tensile strength rate evolution)

But “final” tensile stresses are larger

viscoelastic approach

elastic approach
Benchmark stage 1: MACRO-modelling

Thanks to all the participants

Miguel Azenha & Jose Granja  University of Minho, Portugal

Farid Benboudjema  ENS Paris-Saclay, France

Arnaud Delaplace  LafargeHolcim Research Center, France

Dirk Schlicke & Peter Joachim Heinrich  Technical University of Graz, Austria

Giuseppe Sciumè  University of Bordeaux, France & Stefano Dal Pont  Université Grenoble Alpes UGA, France

Vít Šmilauer & Karolína Hájková  Czech Technical University in Prague, Czech Republic

Vyacheslav Troyan  Kyiv National University of Construction and Architecture, Ukraine
BENCHMARK Stage 1

Stage 1 results presentation

1. Publication in a indexed journal – 2 paper co-authored by participants (MACRO and MICRO)

2. Educational booklet for future generations of engineers and researchers working on modelling of early-age concrete.
BENCHMARK Stage 1

Dissemination:

• Complete benchmark materials openly published in the Internet (Google Drive)
• Personal invitation sent to registered WG2 members (114 participants).
• Open invitation posted on Google+
• Project page set up on Research Gate. Participants invited, 43 followers (in & out Cost Action).
Conclusion and perspectives

• Only example 1 is blind
• Temperature predictions are very close
• Some models are based on constitutive equations which cannot fit evolutions of material parameters,
  ✓ finite element results are no more comparable in the sense of an educational booklet
  ✓ But it is interesting to quantify errors due to the modelling approach
• No significant differences in elastic calculations should be expected if evolutions of material properties are precisely fitted
• A 3rd round is necessary before publishing
• When mechanical results are given, few differences between teams are found
THANK YOU FOR YOUR ATTENTION！
ご清聴ありがとうございました
Go seichō arigatōgozaimashita
MERCI POUR VOTRE ATTENTION

Is cracking due to the shrinkage restraint by the shells, the wall or gradients?