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MODELING OF CONCRETE AT EARLY AGE - BENCHMARK CARRIED OUT WITHIN COST TU 1404

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ABSTRACT

Predicting early-age cracking in concrete structures and its effects on serviceability, such as mechanical performances, durability and tightness, is still a complex task to achieve. Indeed, several complex phenomena occur simultaneously and separation is not straightforward in some cases due to couplings, e.g. coupling of thermal and autogenous strain. The heterogeneity of concrete complicates the analysis of experimental data: e.g. shrinkage occurs only in cement paste and is restrained locally by aggregates. Moreover, for determination of input data it involves a lot of experimental tests (calorimetry, measurements of autogenous shrinkage, mechanical properties, creep in tension etc.) which are not readily available for industrial practice. Therefore, COST Action TU 1404 [1] has been launched. The Working Group 2 of this Action focuses on modeling and numerical simulations. It will allow thus for transferring knowledge from research to the industry in the form of new guidelines and recommendations. The first stage of the benchmark program realized by WG2 has been performed at the microscopic and macroscopic scales. Simple examples have been chosen. The benchmark shows that predicting evolution of thermo-physical and mechanical properties of concrete from its mix design is still a difficult task (microscopic). At the macroscopic scale, the prediction of temperature in massive concrete structures is quite mastered if the model used contains known features such as the thermo-activation process. However, for the prediction of stresses, significant scattering of results has been observed, mainly due to different constitutive equations adopted by the teams for calculation of Young modulus evolution around setting.

Keywords: Early-age, Shrinkage, Creep, Cracking, Benchmark

INTRODUCTION

Cement-based materials (CBM) are the most commonly used construction materials worldwide. Civil engineering structures using CBM are submitted to several types of strains related to drying and hydration of binders. These strains may lead to stresses, and sometimes to cracking, which can reduce durability, mechanical performances and tightness if not precisely addressed in service-life design.

Despite significant research advances that have been achieved in the last decade in early-age testing and simulation of CBM and thereby predicting their service life performance, there have been no generalized European-funded Actions to assure their incorporation into standards available to designers/contractors. Therefore, COST Action TU 1404 [1] has been launched in order to bring together relevant stakeholders (experimental and numerical researchers, standardization offices, manufacturers, designers, contractors, owners and authorities). This will accelerate knowledge transfer in the form of new guidelines/recommendations, introduce new products and technologies to the market, and promote international and inter-

specialty exchange of new information, creating avenues for new developments.

COST Action TU 1404 is divided into 3 Working Groups. The Working Group 1 is called "Testing of cement based materials and RRT+". It focuses on testing of CBM, ranging from the microscopic level, where the microstructure formation of CBM is investigated, up to the development of a set of parameters measured directly on concrete, in addition to those measured on paste and mortar, using the most recently developed techniques, particularly those allowing continuous monitoring. This task will allow building a material database that is especially useful for the simulation models targeted in WG2 to predict the service-life performance.

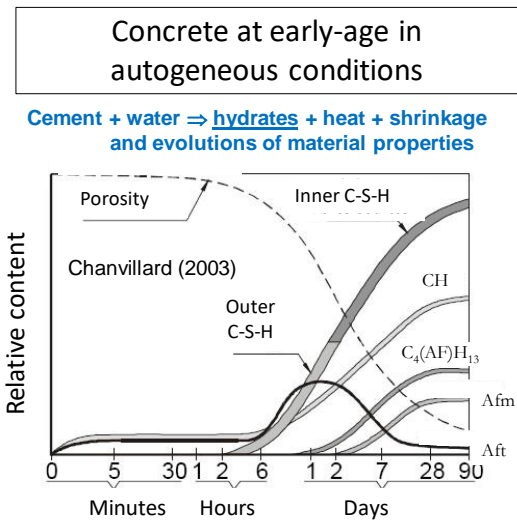
The Working Group 2 is called "Modelling and benchmarking". It focuses on the numerical simulation of the material/structural behavior both at early age and during the service life, and should strongly interact with the results obtained from the Working Group 1. The intricate collaboration between the experimental approaches at several material scales (paste, mortar and concrete) and the corresponding simulation approaches based on multi-scale and multi-physics models are considered

to be one of the added values of this Action. The results of the Working Group will be used to assess the remaining difficulties for the modeling of early-age behavior, and give results for the Working Group 3.

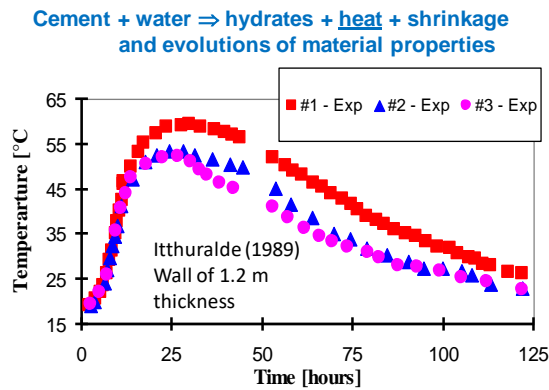
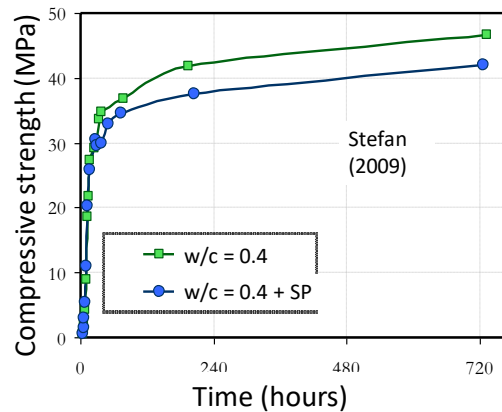
The Working Group 3 is called "Recommendations and products". Its work consists of analyzing different models and capacities, drawing general lessons and proposing standard methodology compatible with the Eurocode standard format to address thermo-hydro-mechanical coupled effects in serviceability design, including transient construction phases. Concurrently, it will address associated material specifications in the material standards and execution provisions in the associated standards.

This paper presents the main objectives of the Working Group 2 and some preliminary results of the benchmark.

DESCRIPTION OF WORKING GROUP 2



Cement + water ⇒ hydrates + heat + shrinkage and evolutions of material properties



Cement + water ⇒ hydrates + heat + shrinkage and evolutions of material properties

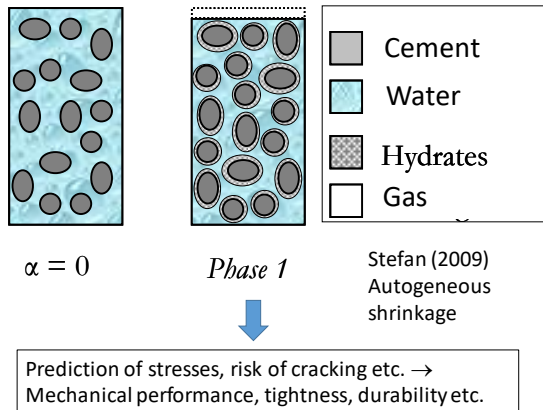


Fig. 1 Phenomena occurring in cement-based materials at early-age.

Description of CBM behavior is a great challenge due to the complex microstructure and various coupled phenomena occurring during setting and hardening (see Fig. 1), in interaction with the environment (relative humidity, temperature). Different modeling approaches exist at various scale levels of concrete microstructure: from atomistic models that focus on molecular size to structural models that describe the behavior of concrete elements, structures and buildings.

The use of complex modeling for predictions of service-life of cement-based materials is usually not required in standards and is quite difficult since it is difficult to identify all material parameters. Moreover, some mechanisms are still controversial (for instance creep, especially the relation between tensile and compressive creep, see Fig. 2) which renders the proposition of relevant and validated models difficult. Instead, simple empirical approaches are often used.

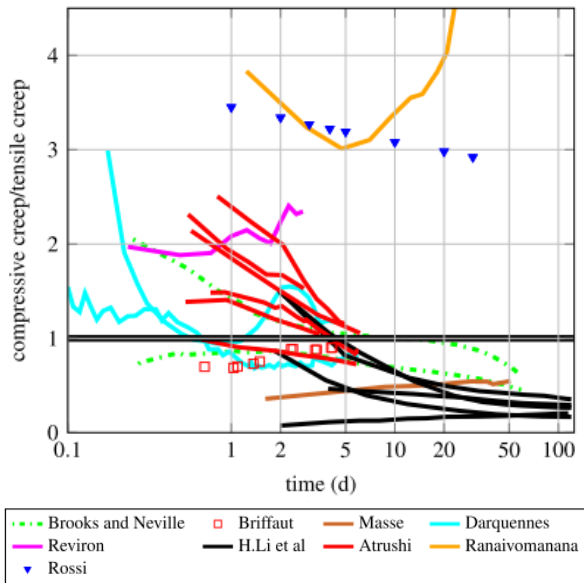


Fig. 2 Evolution of the ratio of the basic compressive creep divided by tensile creep [2].

Hydration of CBM and potential early-age cracking affects mass transport properties (permeability, see Fig. 3 for instance, and diffusivity). It impacts durability (CO₂ and chloride ingress for instance) and tightness (if it is required as in dams, nuclear power plants, radioactive waste containments, sewage treatment plants, etc). This should be also carefully addressed.

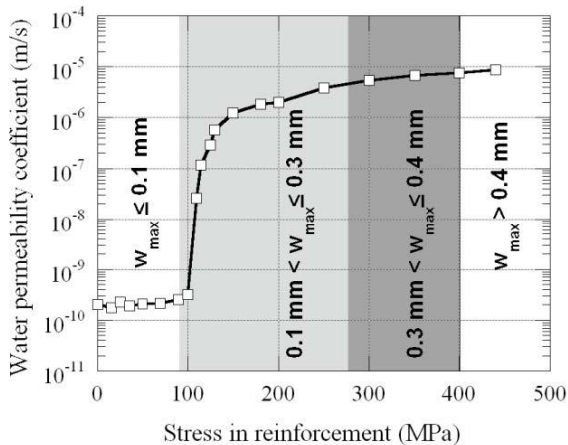


Fig. 3 Evolution of water permeability in a reinforced concrete tie during loading in tension ([7]).

Finally, in order to assess the knowledge (and lacks) regarding modeling of early-age behavior of CBM and numerical simulations of CBM structures, to evaluate the knowledge and to give results to Working Group 3, benchmark activities should also be undertaken.

Six Group Priorities were therefore identified to tackle the issues enlisted above which are summarized below. 113 people have already been

registered in the Working Group 2.

GP2.a - Microstructural modeling

Most of the mechanisms at the origin of cracking in concrete occur in the cement paste. Its microstructure evolves rapidly at early age with the formation of hydration products, the decrease of the total porosity, the reduction of the pores size and the increasing of the tortuosity. The development of mechanical properties, the time-dependent behavior and the transport properties of concrete rely directly on the evolution of the cement paste microstructure. The objectives of this GP are to discuss the most relevant ways of modelling the microstructure development of cement pastes (see Fig. 4 for instance), report recent advances and make comparative reviews of models.

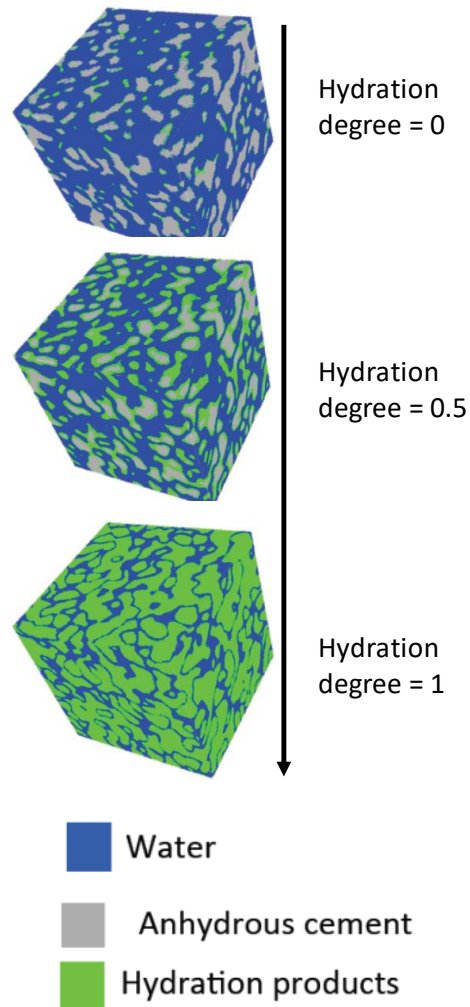


Fig. 4 Example for the description evolution of the microstructure at early-age.

GP2.b - Multiscale modeling

The large variety of cement, additions, etc. as well as the cost and time/devices required for realization of experiments renders optimization of

the concrete mix regarding specifications difficult (material properties, impact on global warming). Virtual testing is an interesting alternative. Starting from the description of the cement paste microstructure (GP2.a), upscaling of material properties must be undertaken up to the concrete scale (GP2.c) (see Fig. 5 for instance). The objectives of this GP are to discuss the most relevant ways to deal with virtual testing, report recent advances and make comparative reviews of numerical strategies (analytical homogenization, finite element calculations, etc.).

GP2.c - Macroscopic modeling

The prediction of cracking in reinforced concrete structures depends not only on the material properties of concrete but also on the mechanical boundary conditions, climate conditions and geometry. Macroscopic models capable of describing time-dependent behavior, transport phenomena and cracking (see Fig. 6 and 7, for instance for the prediction of cracking risk at early-age in massive concrete structures) are thus required. This is important in order to optimize the materials and construction techniques and to interpret data in a monitored structure in a relevant way. These types of multi-physics macroscopic models may be suitable for use in structural design offices (e.g. embedded into finite element software packages). The objectives of this GP are to discuss the most relevant ways to deal with macroscopic modeling, report recent advances and make comparative reviews of modeling strategies (balance equations, mechanics and thermodynamics of porous media, simplified approach, etc.).

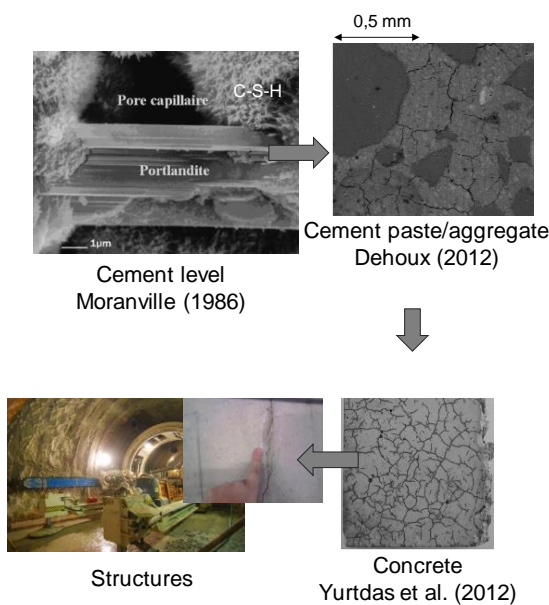


Fig. 5 Example of multi-scale description.

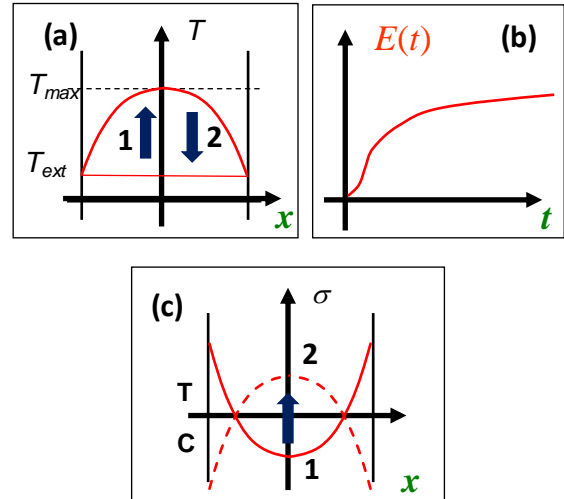


Fig. 6 Evolution of temperature (a), Young modulus (b) and stresses (c), due to the gradient of temperature: large increase of temperature in the core leads to tensile stresses self-equilibrated by compressive stresses in the core. This state of stress reverses during cooling since the Young modulus is greater during this period.

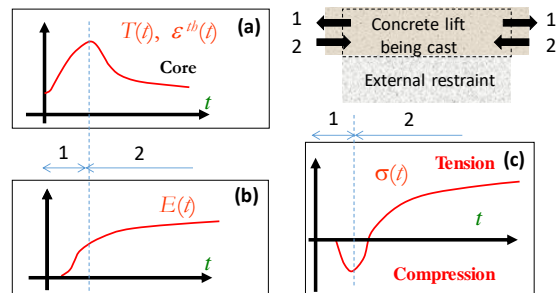


Fig. 7 Evolution of temperature (a), Young modulus (b) and stresses (c), due to external restraint: thermal expansion is restraint during the heating phase, leading to compressive stresses in the current concrete lift. Tension rises during the cooling phase, since the Young modulus is continuously increasing. It can be accentuated by autogenous shrinkage.

GP2.d - Probabilistic modeling

Civil engineering structures are naturally subjected to variability (see Fig. 8, for instance for compressive strength of concrete used for the Millau bridge in France). This variability is due to the natural variability of the constituents of concrete, to errors in constituents weighing, to quality of vibration and compaction, to the initial concrete temperature, to environmental conditions, etc. Probabilistic performance-based approach regarding the service lifetime prediction of concrete structures is thus essential. Since many parameters are involved, a sensitivity analysis could be performed to make relevant choice of probabilistic parameters for the study of uncertainty propagation. It can also be helpful in material and geometry optimization.

The objectives of this GP are to discuss the most relevant ways to deal with probabilistic and sensitivity analysis, report recent advances and make comparative reviews.

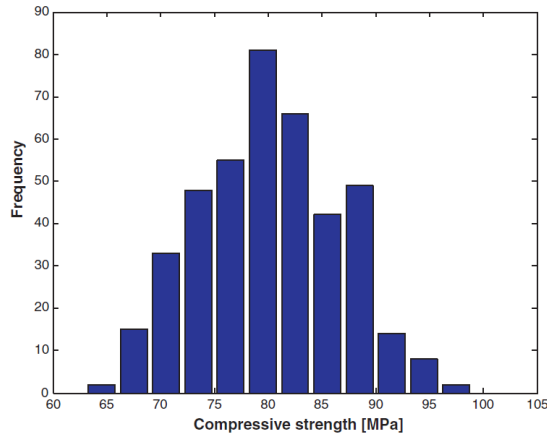


Fig. 8 Compressive strength distribution of the High Performance Concrete of the Millau bridge in France (source: Eiffage Company).

GP2.e - Modeling of transport processes

Many degradation mechanisms are associated with the movement of ions through concrete. Therefore, modelling of transport processes is essential to determine appropriate service-life of concrete structures. This GP focuses on discussing and establishing most appropriate modeling of transport processes through concrete structures. The specific goals of this GP are:

- Establishing a link between models at different scales starting from scale of cement paste microstructure (GP2.a) to determine the transport properties of concrete in conjunction to work of GP2.b.
- Using this link between microstructure and properties of concrete to simulate the chloride transport in concrete (see Fig. 9 for instance).
- Testing predictability of different models for simulating lab scale and field scale chloride transport experiments

The anticipated outcome of this GP is to establish a recommendation for appropriate models for predicting transport properties of concrete and modeling approaches to simulate chloride transport through concrete.

GP2.f - Benchmarking calculations

A fundamental tool for assisting development, understanding and comparison of both micro-scale and macro-scale models mentioned in the

aforementioned GPs are benchmarking tests. It will be possible to evaluate the relative performance of numerical simulation approaches and software (including research and commercial applications) applied to selected real examples of material and structural behavior. Both blind and subsequent non-blind stage of benchmarking have to be included, in relation to the round-robin testing realized in the WG1. The objectives of this GP are to develop relevant strategies for establishment of benchmark studies and compare/analyze the results of different participants in order to propose validation tests and recommendations.

Composition : CEM 1

- $C_3S = 55\% \mid 3,15 \text{ g.cm}^{-3}$
- $C_2S = 18\% \mid 3,28 \text{ g.cm}^{-3}$
- $C_3A = 10\% \mid 3,03 \text{ g.cm}^{-3}$
- $C_4AF = 8\% \mid 3,03 \text{ g.cm}^{-3}$

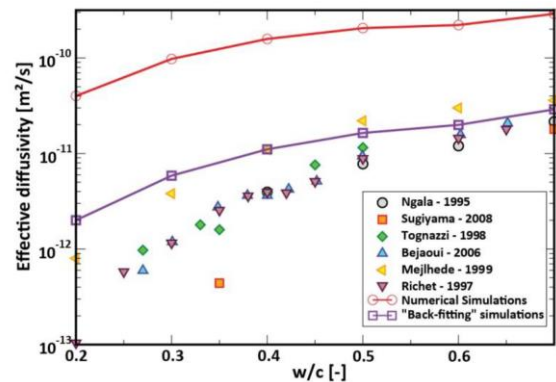
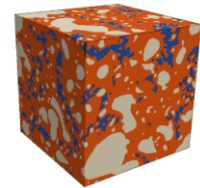


Fig. 9 Evolution of effective diffusivity in cement pastes for different water to cement ratio: comparison between experiments and numerical simulations (bottom) using explicit description of the microstructure (top).

SHORT DESCRIPTION OF THE FIRST STAGE OF BENCHMARK PROGRAM

Three stages of the benchmark program are planned within the COST Action:

- Stage I – simple examples. The idea behind this part of benchmark activities is to serve as a platform to get to know and better integrate different modeling tools used by different participants. The examples to be simulated are fully open, i.e. the participants have access to all input data as well as final results. The examples are based on the published experimental data. The simulations focus both on material properties and

structural phenomena. This stage of the benchmark program has been completed and its results are being analyzed.

- Stage II – extended examples will be studied. Part of the experimental results will be not accessible to the participants to enable blind comparison of the models. The results from the Working Group 1 RRT+ will also be used as examples.
- Stage III – case studies of structural behavior based on field experiments will be used.

The first stage of the benchmark program was divided into macro and micro-meso modelling approaches, which are presented thereafter.

MICRO-MESO EXAMPLE: Hydration evolution, chemical shrinkage and porosity, RH

The example is based on the publication by Wyrzykowski and Lura [4]. The example is aimed at benchmarking microstructural models, but should be also interesting for teams who develop constitutive relationships of cement paste evolution (e.g. influence of water access on hydration).

For the input data, (modified) Bogue composition, Blaine fineness, and other characteristics of the cement ($w/c = 0.3$, CEM I) are provided. Experimental evolutions of different properties at early age are given, and teams should simulate a part or all of these evolutions:

- Hydration heat (isothermal calorimetry),
- Chemical shrinkage (in saturated conditions),
- Pore size distribution at different ages (1 day, 3 days and 7 days) and water porosity at 3 years,
- Sorption isotherm at 7 days,
- RH decrease (self-desiccation),
- Autogenous shrinkage,
- Young and shear modulus, compressive strength.

MACRO EXAMPLE 1: Temperature fields in concrete element

The example is based on the publication by Azenha et al. [5]. The example is aimed at benchmarking macroscopic models predicting temperature evolution in concrete structures.

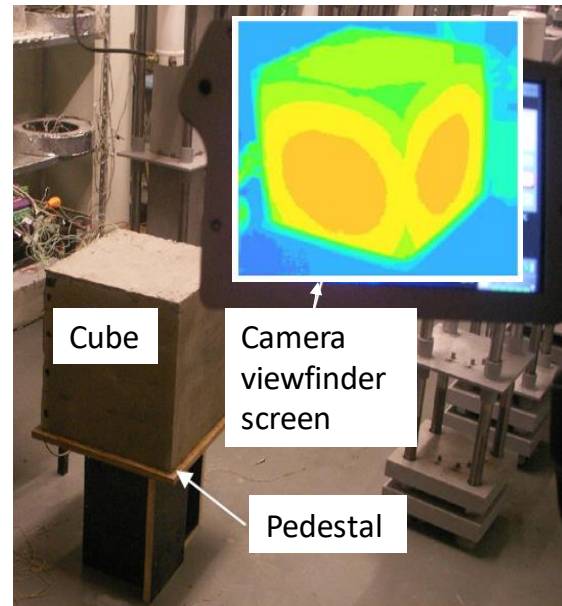


Fig. 10 Specimen and device for the measurement of temperature by thermography [5].

Concrete cube of 400 mm sides was cast and left uncovered at the age of 8.6 h. Temperature evolutions were measured on the surfaces with thermography (see Fig. 10) and inside the element using thermocouples.

As input data, cement type (CEM I), concrete composition, geometry of the cube, environmental conditions (50% RH, 20°C), isothermal calorimetry curves at different temperatures (20, 30, 40, 50, 60°C) are given.

Teams are asked to provide temperature evolutions at the thermocouples location and temperature fields at the surface at specified ages.

MACRO EXAMPLE 2: Temperature and stress fields evolutions

The example is aimed at benchmarking macroscopic models predicting temperature and stresses evolution in a massive wall (thickness of 2 m), in self-restrained conditions (see Fig. 11).

As input data, concrete mix design, evolution of adiabatic temperature, thermal and mechanical properties (from experiments or generated) are provided.

Teams are asked to provide the following evolutions:

- Adiabatic temperature,
- Temperature in the wall,
- Stresses at a Gauss point and in a 2-meters wide wall using elastic or viscoelastic approach.

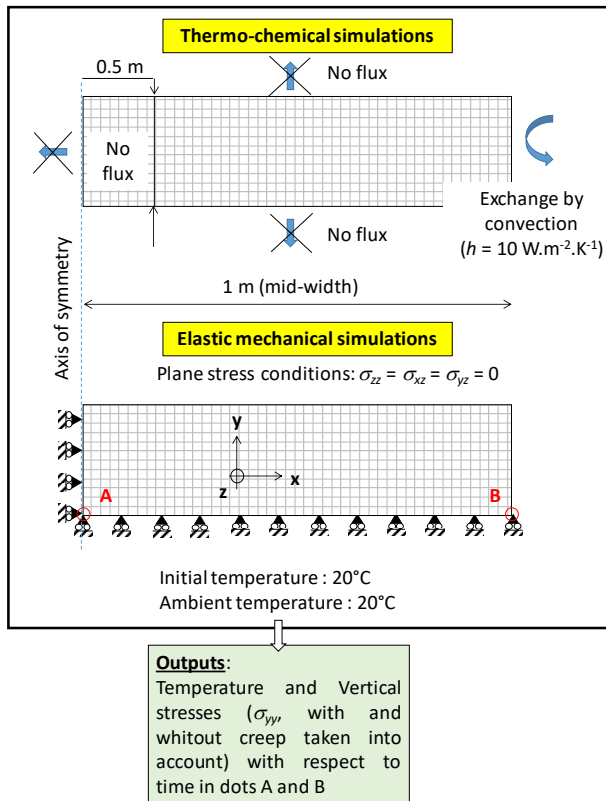


Fig. 11 Description of the geometry and boundary conditions for the 2-meters wide wall.

MACRO EXAMPLE 3: Stresses in a shrinkage restraining device

The example is based on the publication by Turner et al. [6]. The example is aimed at benchmarking macroscopic models predicting cracking risk of a concrete specimen in externally-restrained conditions (see Fig. 12).

As input data, concrete mix design, evolution of adiabatic temperature, temperature in the concrete specimen, thermal and mechanical properties and average stresses (from experiments) are provided.

Teams are asked to provide the following evolutions:

- Temperature in the specimen,
- Stresses in the concrete specimen using elastic or viscoelastic approach.

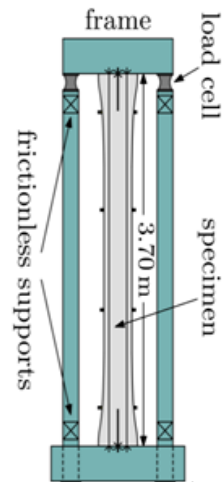


Fig. 12 Sketch of the specimen and the restraining frame.

SOME RESULTS OF THE FIRST STAGE OF BENCHMARK PROGRAM

The number of teams that has participated in the benchmarks is given in the Table 1.

Table 1 Number of teams for each benchmark (first stage)

| Micro | Macro 1 | Macro 2 | Macro 3 |
|-------|---------|---------|---------|
| 7 | 4 | 6 | 3 |

The results are currently being analyzed. Some of them are briefly presented thereafter.

MICRO-MESO EXAMPLE: Hydration evolution, chemical shrinkage and porosity, RH

The evolution of the Young and shear moduli is depicted in Fig. 13. It shows significant differences between the teams, especially for the Young modulus. Several explanations can be given. The evolution of the heat release (and thus hydration degree) was not well reproduced by some teams. Besides, different types of models for hydration as well for the calculation of mechanical properties were used. For instance, for hydration modeling some teams used either analytical equations or voxel description of the cement paste microstructure. For mechanical (elastic) modeling, either homogenization theory or finite element calculations were used. Some fitting (based on the provided experimental data) was also sometimes made by the teams.

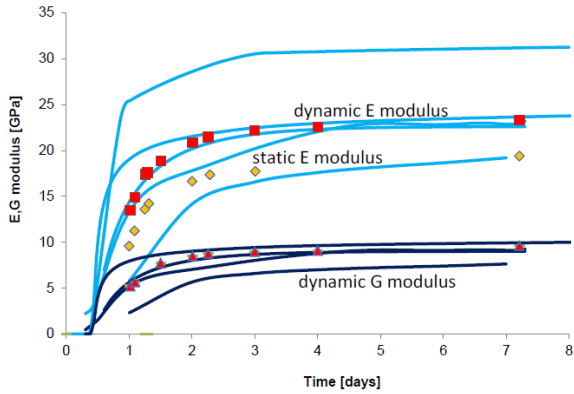


Fig. 13 Evolution of Young and shear moduli in the cement paste.

MACRO EXAMPLE 1: Temperature fields in concrete element

The comparison between experimental and numerical evolution of temperature in a chosen point in a sample is shown in Fig. 14. Team #1 and #2 succeeded to predict correctly the evolution of temperature inside the cube. It was not the case for Team #3 who did not take into account thermo-activation of hydration in their model. It shows, as expected, that this is a key point for prediction of temperature in concrete at early age.

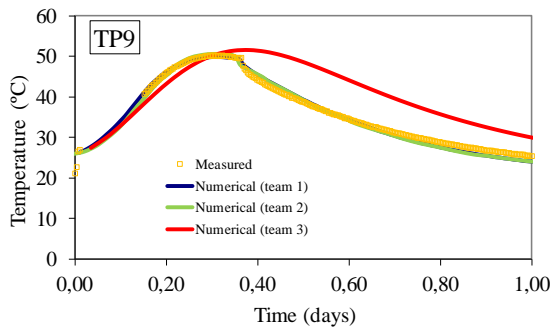


Fig. 14 Experimental and numerical evolution of temperature in the cube.

MACRO EXAMPLE 2: Temperature and stress fields evolutions

Evolution of temperature at the center of a 2-meter wide wall is presented in Fig. 15. All the teams took into account thermo-activation of the hydration process and were able to predict quite correctly the rise of adiabatic temperature for 2 different initial temperatures (see Fig. 16).

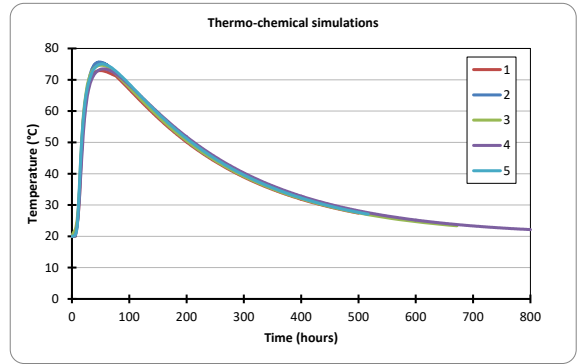


Fig. 15 Numerical evolution of temperature at the center of a 2 meter width wall.

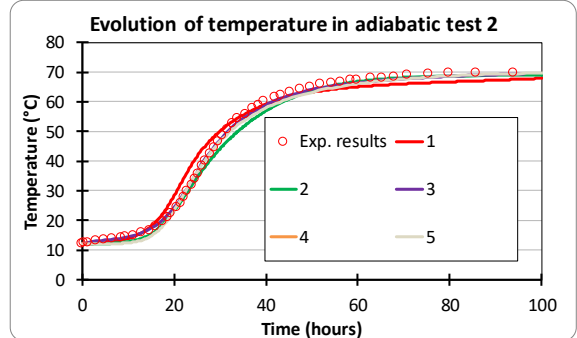
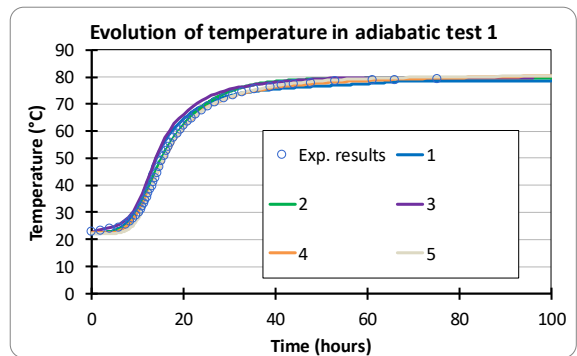


Fig. 16 Evolution of adiabatic temperatures for 2 initial temperatures.

The evolution of vertical stresses at the surface (dot B, see Fig. 11) is shown in Fig. 17, using an elastic approach.

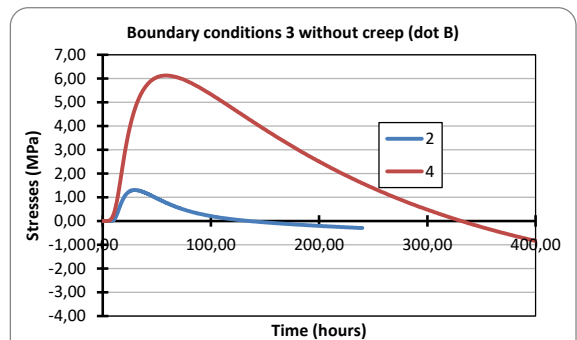


Fig. 17 Evolution of vertical stresses at the surface (dot B, see Fig. 11) in an elastic approach.

The numerical results are similar in terms of trend. The core thermal dilation is restrained by the elements at the surface, which gives rise to compressive stresses in the core self-equilibrated by tensile stresses at the surface. However, the difference of predicted stresses is very large. The main explanation relies on the prediction of Young modulus around the setting point, as revealed in Fig. 9. Indeed, Team #4 predicted a rapid increase of Young modulus before the setting point, which corresponds to the rapid increase of temperature (see Fig. 18). Therefore, Team #4 simulated a large increase of stresses (values higher than the tensile strength). Indeed, the other relevant parameter is autogeneous shrinkage, and the teams have fitted quite well its kinetic and amplitude as shown in Fig. 19.

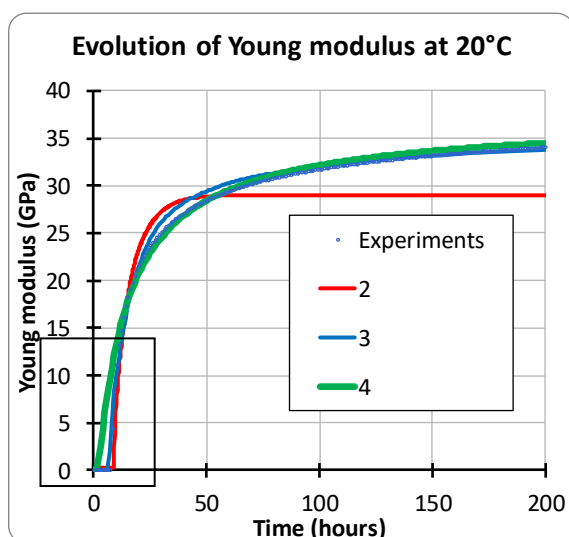


Fig. 18 Evolution of Young modulus at early age.

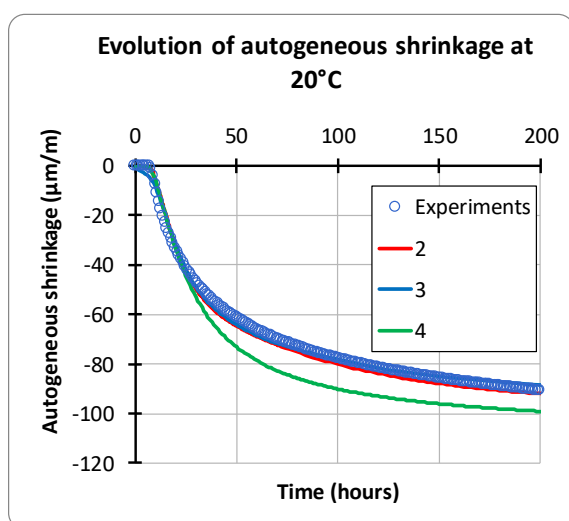


Fig. 19 Evolution of autogeneous shrinkage.

CONCLUSIONS

COST action TU-1404 has been launched in order to bring together relevant stakeholders (experimental and numerical researchers, standardization offices, manufacturers, designers, contractors, owners and authorities) to accelerate knowledge transfer in the form of new guidelines/recommendations, introduce new products and technologies to the market, and promote international and inter-specialty exchange of new information, creating avenues for new developments.

Within this COST action, Working Group 2 has launched 4 benchmarks (first stage, 3 stages are planned) related to prediction of material properties evolution at the cement paste level and temperature/stresses evolution in concrete at early age. The preliminary analysis of the results shows at the macroscopic scale that the prediction of temperature is quite mastered if the model is adequate, i.e., thermo-activation is taken into account. However, the prediction of stresses depends significantly on the capacity to predict the fast evolution of Young modulus just after setting. At the microscopic scale, due to the variety of approaches used for the description of the microstructure and the elastic simulations, significant differences are observed between the teams.

ACKNOWLEDGEMENTS

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