Thermo-mechanical simulations of early-age concrete cracking with durability predictions

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Abstract. Concrete performance is strongly affected by mix design, thermal boundary conditions, its evolving mechanical properties, and internal/external restraints with consequences to possible cracking with impaired durability. Thermo-mechanical simulations are able to capture those relevant phenomena and boundary conditions for predicting temperature, strains, stresses or cracking in reinforced concrete structures. In this paper, we propose a weakly coupled thermo-mechanical model for early age concrete with an affinity-based hydration model for thermal part, taking into account concrete mix design, cement type and thermal boundary conditions. The mechanical part uses B3/B4 model for concrete creep and shrinkage with isotropic damage model for cracking, able to predict a crack width. All models have been implemented in an open-source OOFEM software package. Validations of thermo-mechanical simulations will be presented on several massive concrete structures, showing excellent temperature predictions. Likewise, strain validation demonstrates good predictions on a restrained reinforced concrete wall and concrete beam. Durability predictions stem from induction time of reinforcement corrosion, caused by carbonation and/or chloride ingress influenced by crack width. Reinforcement corrosion in concrete struts of a bridge will serve for validation.

1. Introduction

The term mass concrete describes elements in which high thermal gradients may lead to cracking. Binder content and initial concrete temperature belong to the most critical factors; even concrete members that are only 0.5 m thick may be susceptible to thermal cracking [1]. Significant tensile stresses may develop, leading to early-age thermal cracking, reducing concrete durability [2].

Models for stand-alone temperature prediction in hardening concrete belong among the most traditional concrete models. They consider either adiabatic temperature rise or general thermal boundary conditions [3]-[5]. Humidity transport plays no major role in massive concrete elements; hence only temperature field needs to be calculated. Thermal models can be widened for multiscale formulation, recognizing the role of cement paste for hydration [3]. Precise results can be obtained by first fitting hydration models to semi-adiabatic measurements on small samples and then by upscaling them to a structural scale [6],[7].

Several complex thermo-chemo-mechanical models were formulated during the last decades. They include prediction of stress, often considering concrete creep, autogenous shrinkage, drying shrinkage, and they may predict early-age cracking and crack width [8],[9]. The number of input parameters...
presents the bottleneck of simulations, varying broadly over cements, cement types, local practices and boundary conditions. Nevertheless, growing computer power and calibrated material laws allow simulating various concrete structures. The simulations of the massive concrete structures are in the focus of this paper. These simulations use a thermo-(chemo-)mechanical model implemented in an open-source finite element package OOFEM [10].

2. Thermal model

Temperature field on a block is predicted from heat balance equation

\[-\nabla^T q(x) + \overline{Q}(x,t) = \rho(x) c_v(x) \frac{\partial T(x,t)}{\partial t}\]

using further Fourier’s law on an isotropic material

\[q(x) = -\lambda(x) \nabla T(x)\]

where \(T(x,t)\) stands for temperature, \(Q(x,t)\) for heat power from hydrating cement (W/m\(^3\)), \(\rho(x)\) for concrete density (kg/m\(^3\)), \(c_v(x)\) for concrete thermal capacity (J/kg/K), and \(\lambda\) for heat conduction (W/m/K). Equation (1) can be further complemented with initial conditions and several other boundary conditions including convection. Here, thermal radiation is neglected.

The heat power \(Q(x,t)\) originates from hydrating cement paste according to Figure 1. The figure defines material scale with an affinity hydration model that captures reaction kinetics. Since the affinity model depends strongly on temperature, coupling with structural scale needs to be carried out. The model uses a strong coupling with a predictor-corrector scheme to achieve balance on both scales.

Affinity hydration model is the heart of the multiscale formulation. The evolution of hydration is approximated with a four-parametric function

\[\dot{A}_{25} = B_1 \left( \frac{B_2}{\alpha_\infty} + \alpha \right) (\alpha_\infty - \alpha) \exp\left(-\frac{\alpha}{\alpha_\infty}\right)\]

where \(\dot{A}_{25}\) is the affinity at isothermal temperature 25°C, and \(B_1, B_2, \alpha_\infty, \alpha\) are the four parameters for calibration. Isothermal calorimetry is a perfect method how to obtain these parameters. Figure 2 shows released heat of common cements [6]. As described in Figure 1, temperature influences hydration rate and vice versa. Temperature-dependent kinetics is approximated with Arrhenius equation.
\[
\frac{1}{Q_{h,\text{pot}}} \frac{\partial Q_h}{\partial t} = \frac{\partial \alpha}{\partial t} = A_{25} \exp \left[ \frac{E_a}{R} \left( \frac{1}{T_{25}} - \frac{1}{T} \right) \right]
\]  

where \(Q_{h,\text{pot}}\) is the potential hydration heat (J/g), \(E_a\) the activation energy and \(R\) the universal gas constant. This multiscale heat transfer model has been used several times for validation with excellent results on structures with volume from 0.01 m\(^3\) up to 1050 m\(^3\) [6].

3. Mechanical model
The mechanical part combines extended B3 creep model [11] with an isotropic damage model. The incremental constitutive equation reads

\[
\Delta \sigma_{\text{eff}} = \tilde{E} D_\nu (\Delta \varepsilon - \Delta \varepsilon'' - \Delta \varepsilon_{\text{sh,aut}} - \Delta \varepsilon_T)
\]

where \(\Delta \sigma_{\text{eff}}\) is an increment of effective stress, \(\tilde{E}\) incremental elastic modulus, \(\Delta \varepsilon\) strain increment, \(\Delta \varepsilon''\) strain increment due to creep, \(\Delta \varepsilon_{\text{sh,aut}}\) an increment of autogenous shrinkage, \(\Delta \varepsilon_T\) thermal strain increment [11][16]. \(D_\nu\) stands for a unit elastic stiffness matrix. Using the concept of damage mechanics, the nominal stress is computed as

\[
\sigma = (1 - \omega) \sigma_{\text{eff}}
\]

where \(\omega\) is a scalar damage. Cracking is initiated when the effective principal tensile stress exceeds the tensile strength of concrete. Exponential softening is assumed with a crack-band approach to maintain objectivity with respect to the finite element size [10]. Evolution of compressive strength, tensile strength and fracture energy is adopted from ModelCode 2010 [15] and the user can directly enter concrete strength at 28 days. Autogenous shrinkage is controlled by maximum asymptotic value and the evolution can be specified according to ModelCode 2010 [15] or B4 model [16]. The crack width \(w\) is evaluated as

\[
w = L_{ch} \omega \varepsilon_{1,\text{red}}
\]

where \(L_{ch}\) stands for element length projected in direction of the first principal stress and \(\varepsilon_{1,\text{red}}\) is the first principal strain decreased by thermal and autogenous strain.

A staggered approach is adopted; the thermal part of the analysis passes temperatures to the mechanical part. A user can define the end of setting time (4 hours by default) and the beginning of mechanical analysis (8 hours by default).

4. Thermo-mechanical validations

4.1. Temperatures on Sri Lanka’s foundation caps
A new commercial/residential building Access Tower II with 28 floors has been constructed during 2014-2016. There have been several pile cap foundations, the biggest one with dimensions of 16.0 × 8.0 × 2.5m. Technical standards specified maximum concrete temperature of 70°C with compressive strength over 45 MPa at 28 days. After concrete mix optimization, 395 kg/m\(^3\) of fly ash cement was used. A pile cap with dimensions of 7.15 × 7.15 × 2.5 m was validated via gage T3 which is located 125 mm from the concrete surface as indicated in Figure 3. The maximum measured temperature in T1 was of 70.1°C while the model predicted 72.7°C. Thermal gages served also in other two pile caps with slightly different dimensions, yielding maximum temperature differences 2.2 and 1.6°C.
4.2. Simulation of Oslo’s restrained wall

The Norwegian Public Roads Administration developed a “low-heat” concrete with a minimal risk of early-age cracking with a forerunner experiment for Bjørvika submerged tunnel project running between 2005 and 2012. A reference concrete SV 40 with CEM I 52.5 404 kg/m$^3$ and silica fume 20 kg/m$^3$ was tested from a series of small-scale lab tests to a restrained wall [17]. The first test was a small semi-adiabatic calorimeter using a concrete cube with 247 mm edge wrapped in EPS foam. The cement used in this test had slightly higher initial kinetics than that of similar cement in the database [6]; hence, the kinetic was slightly accelerated to match core temperature in the adiabatic calorimeter, see Figure 4. A restrained wall with the same concrete composition was built in Oslo, see Figure 5. In particular, the right wall utilized low-heat concrete with a minimal risk of early-age cracking and high water tightness, whereas the left wall utilized SV40 concrete for comparison. Both walls were cast on a hardened raft concrete slab [17] and the left wall is validated.

Thermal simulation is carried out on a wall with a cross section of 1.0 × 2.0 m. The length was shortened to 6.5 m to decrease computing time. The next reduction came from symmetry so the modeled block size shrank to 0.5 × 2.0 × 3.25 m.

**Figure 3.** Top view of foundation caps, temperature validation in gage T3 and temperature field in a characteristic cap.

**Figure 4.** Core concrete temperature is a semi-adiabatic calorimeter.

**Figure 5.** A restrained wall in Oslo [17].
Figure 6. Temperature field during maximum temperature at 30 hours (left) and validation (right).

A fixed temperature of 15°C was assigned to the bottom surface and fluctuating ambient temperature ranging 12-18°C was prescribed to the remaining surfaces. Heat transfer coefficients set at 4.50 W/m²/K acted on vertical surfaces covered with a formwork while the top was covered with a foil yielding a heat transfer coefficient of 13.50 W/m²/K. Figure 6 shows temperature validation in gage 15, located in the middle of the wall and 1.2 m from the bottom. Formwork was removed after 216 hours from mixing time and the formwork stripping down was neglected in the simulation.

The mechanical part used B3 creep model for concrete with Microprestress-Solidification extension [11]. A mean compressive concrete strength was set at 77 MPa, ultimate autogenous shrinkage -180 µε, and the coefficient of thermal expansion taken 10·10⁻⁶ K⁻¹ as the average [17]. Reinforcement ratio was estimated as 0.002 which had a small effect on mechanical behavior but improved convergence. It was assumed that the hardened concrete was fully restrained at the bottom of the simulated wall.

The simulation shows that first cracks on the surface appeared already 12 hours after casting but they closed at 60 hours due to surface cooling. The majority of the cracks appeared after 70 hours on the interface with the hardened concrete base where a high shear stress leads to tension on inclined planes. Figure 7 shows cracks and principal stress at t=300 h, where the widest cracks attain width of 0.58 mm. The validation of horizontal strain measured by vibrating wire strain gage is in agreement with experimental data, see Figure 7.

Figure 7. First principal stress and cracks at 300 hours. Validation of horizontal strain.
5. Extension for durability

Presence of cracks accelerates both carbonation and chloride ingress. Carbonation depth can be computed from Papadakis and Tsimas’s model [18], which reads

\[ x_c = \sqrt{\frac{2D_{c,CO_2}CO_2}{0.218(C+kP)}} \sqrt{t} = A_t \sqrt{t} \]  

and the acceleration due to crack width can be computed with Kwon and Na’s model [19]

\[ x_c(t) = (2.816\sqrt{w} + 1)A_t \sqrt{t} \]

where \( w \) is the crack width (mm). Note that the presence of a 0.3 mm wide crack increases carbonation depth by a factor of 2.54. This also means that the induction time is 6.46 times shorter compared to a sound concrete.

The model for chloride ingress is based on Kwon et al. [19] as 1-D transient problem with initially chloride-free content

\[ C(x,t) = C_s \left[ 1 - \text{erf} \left( \frac{x}{2\sqrt{D_m(t)f(w)t}} \right) \right] \]

where \( C_s \) is the chloride content at surface (kg·m\(^{-3}\)), \( D_m \) is the averaged diffusion coefficient at time \( t \) (mm\(^2\)s\(^{-1}\)), \( x \) is the position from the surface in mm and \( f(w) \) gives the acceleration by cracking (equals to one for a crack-free concrete). Based on recent results, the following scaling function is proposed (Kwon, Na et al. 2009)

\[ f(w) = 31.61w^2 + 4.73w + 1 \]

where \( w \) stands for crack width (mm). The presence of a 0.3 mm crack increases the mean diffusion coefficient by a factor of 5.26. In reality, crack width evolves and incremental solution needs to be formulated. Several examples for carbonation and chloride ingress were already presented in [20].

6. Conclusions

Performance of thermo-(chemo)-mechanical model was demonstrated on several mass concrete structures. Generally speaking, temperature predictions show excellent accuracy, with the error falling usually below 3°C. Mechanical part needs more accurate definition of boundary conditions and contains several parameters in the constitutive laws. Current simulations disregard drying which would become more important in thinner concrete elements. We demonstrated reasonable predictions on a restrained wall with crack localization and extension to durability considering carbonation or chloride ingress.

Acknowledgements

We acknowledge collaboration with LafargeHolcim R&D, providing valuable temperature measurements and technical details for validations. The financial support from the Technology Agency of the Czech Republic under the project CESTI TE01020168 is also gratefully acknowledged.

References

[1] Neville A M 1997 Properties of Concrete (London: Wiley)
[2] Weiss W, Yang W and Shah S 1999 Factors influencing durability and early-age cracking in high strength concrete structures Proc High Performance Concrete: Research to Practice (Farmington Hills, MI) pp 387–409
[3] Bentz D P, Waller V, and de Larrard F 1998 Prediction of Adiabatic Temperature Rise in Conventional and High-Performance Concretes Using a 3-D Microstructural Model *Cement and Concrete Research* **28** pp 285–297

[4] Estrada C F, Godoy L A, and Prato T 2006 Thermo-mechanical behavior of a thin concrete shell during its early age *Thin-Walled Struct* **44** pp 483–495

[5] Park K-B, Jee N-Y, Yoon I-S and Lee H-S 2008 Prediction of Temperature Distribution in High-Strength Concrete Using Hydration Model *ACI Mater. J.* **105** pp 180–6

[6] Leal Da Silva W, Šmilauer V and Štemberk P 2015 Upscaling semi-adiabatic measurements for simulating temperature evolution of mass concrete structures *Materials and Structures* **48** pp 1031-41

[7] Briffaut M, Benboudjema F, Torrenti J-M and Nahas G 2012 Analysis of semi-adiabatic tests for the prediction of early-age behaviour of massive concrete structures *Cement and Concrete Composites* **34** pp 634–641

[8] Gawin D, Pesavento F and Schrefler BA 2006 Hygro-thermo-chemo-mechanical modelling of concrete at early ages and beyond Part I: hydration and hygro-thermal phenomena *International Journal for Numerical Methods in Engineering* **67** pp 299–331

[9] Gawin D, Pesavento F and Schrefler BA 2006 Hygro-thermo-chemo-mechanical modelling of concrete at early ages and beyond Part II: shrinkage and creep of concrete *International Journal for Numerical Methods in Engineering* **67** pp 332–363

[10] Patzák B 2012 OOFEM - an object-oriented simulation tool for advanced modeling of materials and structures *Acta Polytechnica* **52** pp 59–66

[11] Jirásek M and Havlásek P 2014 Microprestress-solidification theory of concrete creep: Reformulation and improvement *Cement and Concrete Research* **60** pp 51–62

[12] Hellmich C, Mang HA and Ulm F-J 2001 Hybrid method for quantification of stress states in shotcrete tunnel shells: combination of 3D in situ displacement measurements and thermochemoplastic material law *Computers & Structures* **79** pp 2103–15

[13] Jendele L, Šmilauer V and Červenka J 2014 Multiscale hydro-thermo-mechanical model for early-age and mature concrete structures *Advances in Engineering Software* **72** pp 134–146

[14] Ulm F-J and Coussy O 1998 Couplings in early-age concrete: From material modeling to structural design *International Journal of Solids and Structures* **35** 4295–4311

[15] Fédération Internationale du Béton 2010 Model Code 2010 *FIB Bulletin International Federation for Structural Concrete* **55**

[16] RILEM Technical Committee TC-242-MD 2015 Model B4 for creep, drying shrinkage and autogenous shrinkage of normal and high-strength concretes with multi-decade applicability *Materials and Structures* **48** 753–770

[17] Ji G 2008 *Cracking risk of concrete structures in the hardening phase: Experiments, material modeling and finite element analysis* (NTNU Trondheim)

[18] Papadakis V G and Tsimas S 2002 Supplementary Cementing Materials in Concrete Part I: Efficiency and Design *Cement and Concrete Research* **32** 1525–1532

[19] Kwon S J et al 2009 Service Life Prediction of Concrete Wharves with Early-aged Crack: Probabilistic Approach for Chloride Diffusion *Structural Safety* **31** 75-83

[20] Šmilauer V, Jendele L and Červenka J 2013 Prediction of Carbonation and Chloride Ingress in Cracked Concrete Structures *Proceedings of the Fourteenth International Conference on Civil, Structural and Environmental Engineering Computing Stirling* (Civil-Comp Press Ltd) pp 1-12