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ANALYSIS OF CONCRETE FOUNDATION – HEAT CONDUCTION MULTISCALE MODELING

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Summary: *Temperature evolution in concrete constructions due to hydration heat presents a formidable problem causing early age cracking and from the chemical point of view changing a hydration kinetics. Cement hydration model was incorporated in the finite element program, coupling hydration heat with actual temperature in a heat-conduction problem. The hydration model runs at the micrometer level and allows to compute local quantities, e.g. heat of hydration, degree of hydration, or homogenised elastic properties. Such tool is used to validate concrete slab member casted at nine stages and showing the evolution of temperature.*

1. Introduction

Hydration of Portland cement is an exothermic process, releasing significant amount of heat, typically up to 500 J/g of cement. The heat evolution can be attributed to the reaction of the most common mineral $\mathrm{C_3S}$ of Portland cement with the equation

$$\mathrm{C_3S(1) + 5.3H(1.34) \rightarrow C_{1.7}SH_4(1.52) + 1.3CH(0.61),\ 517\ J/g\ of\ C_3S} \tag{1}$$

where the number in parenthesis represent the volume of constituents when the reaction proceeds under 20°C. The temperature rise inside the concrete structure is critical in massive structures since the surface area fraction decreases with volume thus a cooling from surrounding environment is reduced. The thermal stress may cause structural cracking when the tensile stress is exceeded, the cracks often penetrate through the whole section, are wider and often irreversible [Maekawa et al., 1999]. It is a known fact that the kinetics of hydration is strongly influenced with actual temperature, as a rule of thumb, being doubled with the temperature rise of 10°C. For the proper simulation of cement and concrete hydration, following factors at the micrometer scale should be taken into account:

- particle size distribution of cement,
- chemical composition of cement ($\mathrm{C_3S}$, $\mathrm{C_2S}$, $\mathrm{C_3A}$, $\mathrm{C_4AF}$, gypsum),

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- actual temperature and its history,
- water regime (saturated and sealed conditions),
- the water-to-cement ratio (*w/c*) and the amount of cement in concrete.

2. Cement hydration model

The hydration model CEMHYD3D was presented at previous conference together with the calculation of effective elastic properties [Šmilauer, 2005, Šmilauer and Bittnar, 2006]. The microstructure of cement paste, referring to as a representative volume element (RVE), is modeled in a discretized form of voxels. Each voxel represents one chemical phase with the size of 1 × 1 × 1 μm. The RVE is reconstructed with the help of cement fineness. The reactions are modeled on the basis of cellular automaton, describing the process of dissolution, transport, nucleation, and reaction.

Since the amount of reacted voxels is known from chemical reactions, the liberated heat may be calculated from evolving microstructure [Bentz et al., 1999]. At the current stage, no moisture transport and its effect on hydration is considered. The temperature effect on hydration kinetics is determined from Arrhenius equation for all implemented reactions, where the characteristic time τ is modified according to the maturity principle [Maekawa et al., 1999]

$$\tau(T) = \tau(T_0) \exp\left[\frac{E_a}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right], \tag{2}$$

where T and T_0 are arbitrary and the reference model temperature (25°C) of reactions, R is the universal gas constant (8.314 Jmol^{-1}K^{-1}) and E_a is the apparent activation energy, typically 40 kJmol^{-1} for ordinary Portland cement [Kada-Benameur et al., 2000].

The rules of dissolution, collision and nucleation, handled with the help of the cellular automata, represent unfortunately no meaningful scale of time. Original linear mapping of cycles to time show considerable disagreements with experiments [Bentz, 2000]. Parabolic mapping, based on the Knudsen's parabolic dispersion model, was found appropriate under different curing conditions and cement types [Bentz, 1995]. Knudsen's model assumes that the diffusion of ions takes the control over the hydration rate with the dormant period lasting t_0

$$\text{time} \;=\; t_0 + \beta\, \text{cycle}^2. \tag{3}$$

The parameter β is usually found in the interval $1 \cdot 10^{-4} \leq \beta \leq 1.1 \cdot 10^{-3}$ [Bentz, 1995, Bentz et al., 1999]. The CEMHYD3D model requires two parameters for proper calibration, i.e. t_0 and β from Eq. (3). Parameter t_0 represents the latency of dormant period influenced by superplasticizers, alkalies, parameter β controls the overall kinetics.

3. Multiscale heat conduction model

Non-stationary heat conduction problem may be formulated with the following equation

$$\begin{aligned} -\nabla^T \mathbf{q}(\mathbf{x}) + Q(\mathbf{x}, t) &= \rho(\mathbf{x}) c_v(\mathbf{x}) \frac{\partial T(\mathbf{x}, t)}{\partial t}, & (4)\\ \mathbf{q}(\mathbf{x}) &= -\lambda(\mathbf{x}) \nabla T(\mathbf{x}), & (5) \end{aligned}$$

where $\mathbf{q}(\mathrm{x})$ is a heat flux, $Q(\mathrm{x}, t)$ represents a heat source, $\rho(\mathrm{x})$ stands for a material density, $c_v(\mathrm{x})$ is a specific heat capacity and $\lambda(\mathrm{x})$ is a heat conductivity of isotropic material. Dirichlet, Neumann and Cauchy boundary conditions and initial boundary conditions may be associated with Eq. (4). The principle of virtual temperatures allows numerical solution of Eq. (4) via FEM and time discretization resulting to explicit or implicit time discretization, for example. The heat source $Q(\mathrm{x}, t)$ represents the hydration heat of concrete, which is determined from the CEMHYD3D model of cement hydration and strongly influenced by surrounding temperature. Therefore, it is necessary to couple hydration model at the microscale with the structural model at the macroscale in terms of temperature and hydration heat, Fig. 1. An open-source package TRFEL was used for the structural level. It is possible to assign the same material model of cement to several finite elements in the case that the temperatures within these elements do not vary significantly.

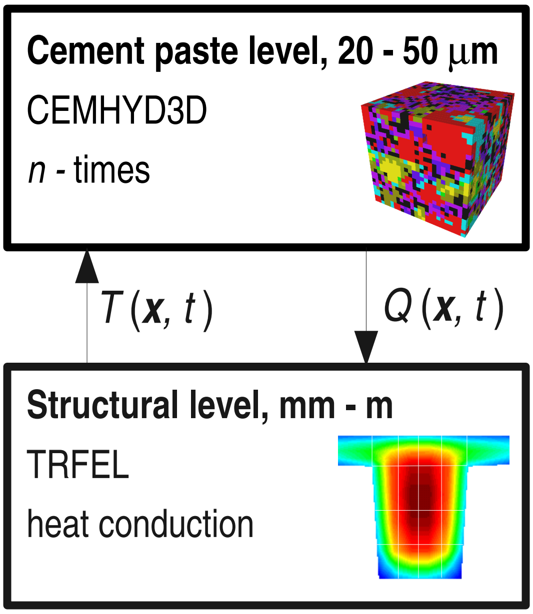

Figure 1: Coupling between two levels; hydration heat produced at the cement paste level controlled with temperature at the structural level.

4. Validation of calorimetry data on isothermally cured cement paste

The hydration model must be calibrated for the cycle mapping to the real time according to Eq. (3). Reference ordinary Portland cement 42.5 R produced at location Mokrá with known chemical composition and parameters was used for the model calibration at *w/c* $= 0.5$. Isothermal calorimetry data at 25°C were calibrated to CEMHYD3D model with the RVE size of 50 $\times$ 50 $\times$ 50 μm. The results are in Fig. 2. Small discrepancy is observed at the beginning of hydration due to model assumptions of C-S-H control over kinetics, the main accelerating period is modeled properly. A discrepancy of later hydration stage may be attributed to the sensitivity and stability of the calorimeter. Potential hydration heat corresponds to 520.54 J/g of cement. The calibration gives $\beta = 7.8 \cdot 10^{-4}$ and $t_0 = 1.2$ h.

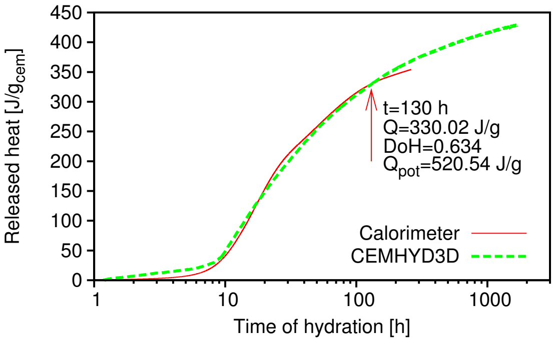

Figure 2: Evolution of hydration heat in plain cement paste *w/c* $= 0.5$; measured in isothermal calorimeter at $25°\mathrm{C}$ and calibrated simulation from CEMHYD3D model.

5. Validation of the concrete slab

Foundation slab of 1 m thickness is situated in the administration building at Těšnov in Prague. Thermometers were installed in a characteristic cross section, shown in Fig. 3. The slab was casted in several steps; in the region of installed thermometers three layers of concrete were placed. The time delay between individual placing was three hours. After the final casting, the lower part of slab was covered with a plastic foil to prevent evaporation. Other parts of slab were casted after approximately one month.

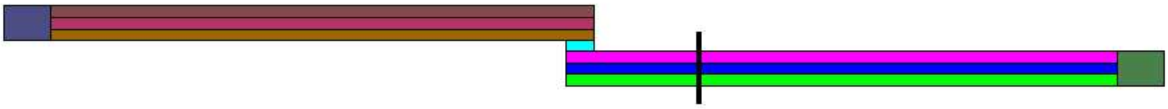

Figure 3: Domains of cement hydrating materials in a cross section area of concrete slab, black line corresponds to the position of thermometers.

Known concrete composition is given in Tab. 1. Although CEMHYD3D may handle the hydration of slag cement directly, the modeling was considered on a pure Portland cement due to unknown parameters of slag. Generally, blast furnace cement is produced from Portland cement, where 21 - 35 % of cement mass is replaced by furnace slag. It was assumed 25 % replacement, i.e. 315 kg/m^3 of pure remaining Portland cement with assumed clinker composition of C_3S 60 %, C_2S 20 %, C_3A 10 %, and C_4AF 10 % by volume and with assumed typical Blaine fineness of 350 m^2/kg. Fresh concrete had the specific density of 2422.5 kg/m^3 and *w/c* $= 0.43$. Sealed conditions for the hydration modeling were assumed, corresponding well to the real concrete curing. The potential hydration heat of cement was calculated from CEMHYD3D model as $Q_{pot} = 513$ J/g.

Two dimensional heat conduction problem was solved on the slab cross section in Fig. 3. The integration time step of Eq. (4) was set to 10 minutes up to three days of hydration, than extended to 100 minutes using Crank-Nicholson scheme. The simulation considered growing structure when additional layers of fresh concrete were casted according to the time schedule. The amount of DOF was 61029, covering 19848 elements when all parts of slab were turned on. The elements were grouped to nine hydrating cement materials according to layers shown

Table 1: Concrete composition used in the simulation of the slab, *w/c* = 0.43.

Cement parameter	Value
Type	B40/90-V8
Cement II-B-S 32.5	420 kg/m^3
Water	180 kg/m^3
Fine aggregates	750 kg/m^3
Coarse aggregates	960 kg/m^3
Fly ash	20 kg/m^3
Admixtures	2.3 kg

in Fig. 3. It was further assumed that concrete had the specific heat capacity $c_v = 810$ Jg^{-1}K^{-1}, the heat conductivity $\lambda = 1.5$ Wm^{-1}K^{-1}, and the parameters $\beta = 2.5 \cdot 10^{-4}$, $t_0 = 0$ h.

The temperature evolution is depicted in Fig. 4 for the middle and the higher point in the position of thermometers. The middle point was located 0.5 m from the inferior surface of slab while the top point at 0.8 m. The results revealed excellent predictions up to approximately 48 hours of hydration. At that time, the degree of hydration is at least 0.59 and the hydration does not produce significant amount of the heat anymore. By our opinion, the discrepancy of later stages may be attributed to the climate conditions which were included as average values for Prague, corresponding to considered period of time. In addition, slow reaction of slag in the cement may release some additional heat that was not taken into account.

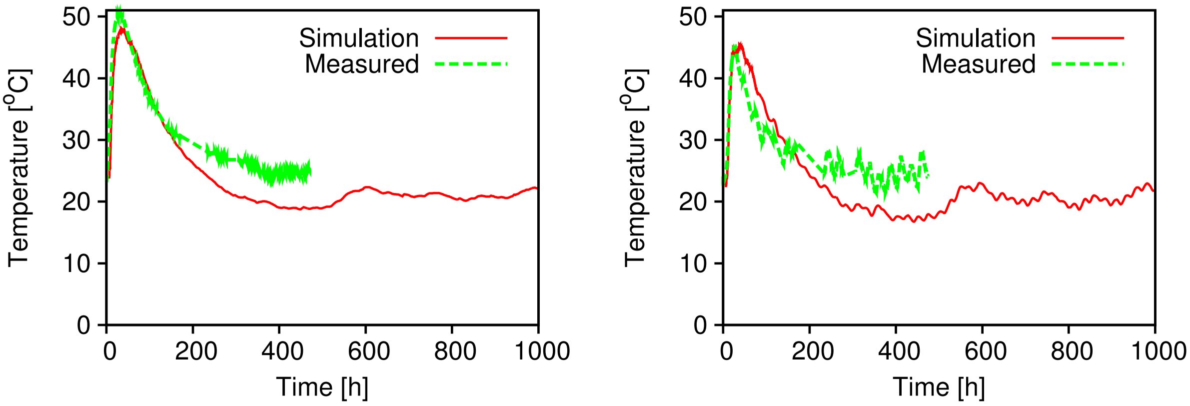

Figure 4: Temperature evolution at the position of thermometers; in the middle of the slab (left) and 0.8 m from the bottom part (right).

6. Conclusion

This paper has presented a multiscale approach for a heat conduction problem, validated for the concrete slab with corresponding climatic and boundary conditions. The slab was casted in nine steps. Such multiscale analysis allows to explore the effects of cement composition, cement fineness, curing regime, or initial hydrating temperature on the structural member. The simulation revealed substantial temperature increase in the massive part of the slab foundation.

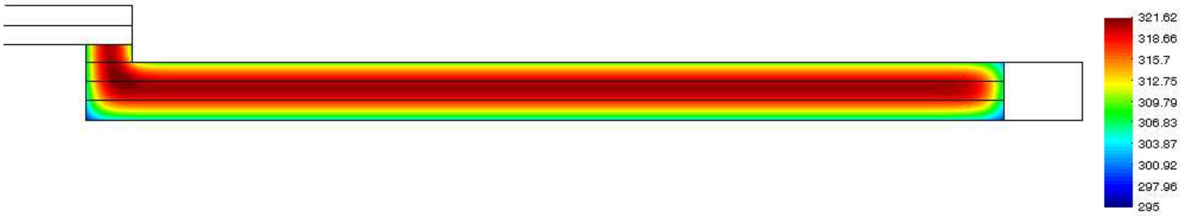

Figure 5: Temperature distribution in the lower part of slab at 33 hours from the beginning of simulation, in Kelvin.

7. Acknowledgement

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8. References

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