Early-age heat flow and hydration in cementitious composites: numerical modelling based on temperature measurements

E Martinelli¹, M Pepe² and C Lima³

¹ Associate Professor, Department of Civil Engineering, University of Salerno, Italy
² Research Assistant, Department of Civil Engineering, University of Salerno, Italy
³ Head of Modelling section, TESIS srl, Fisciano (SA), Italy

e-mail: mapepe@unisa.it

Abstract. The heat generated during early age cement hydration causes a semi-adiabatic temperature rise of hardening concrete, while starting to develop its physical and mechanical properties. As a matter of principle, the heat generated by the hardening mixture depends on the cement properties and its hardening conditions like for instance the type of binders, quality of aggregates, water-to-cement ratio and type of formwork. A simple 1D numerical model can be formulated for simulating the evolution in time of this reaction, in order to identify the so-called degree of hydration. The present paper proposes a detailed description of a theoretical approach which allow to assess the temperature development occurring in concrete elements at the early-age when the produced mixture is cured in semi-adiabatic boundary conditions. In this numerical procedure, the differential heat equation takes into account the heat that liberates to the environment through the formwork or concrete’s surface. This is done by considering the Arrhenius Principle and assuming a pre-defined shape of the adiabatic hydration curve of the concrete mixture. Hence, an indirect identification procedure of the aforementioned adiabatic curve is ideally carried out, as the simulated temperature evolution in semi-adiabatic conditions is brought to match the temperature measurements on a hardening concrete sample. This modelling procedure, enabling various boundary conditions, ranging from semi-adiabatic to isothermal, can be used to calculate the degree of hydration of a real in-situ cast concrete. Specifically, considering the variation of concrete strength class and element size some possible applications are proposed: this represents a simplified approach for the prediction of the temperature time-evolution in the concrete elements at early-age which may be also used as a practical tool for mitigating the risk of premature cracking.

1. Introduction
The mechanisms governing the evolution of the setting and hardening processes for cementitious composites are, generally, identified through the identification of the Degree of Hydration (DoH) [1]. In addition, the DoH is directly correlated to the physical and mechanical properties’ development, at the early-age, for the concrete mixture under investigation. [2]. On the other hand, it is worth to mention that the determination of the degree of hydration result to be easily evaluable only in the case in which the setting and hardening processes occurs in adiabatic condition, since the resulting DoH is directly proportional to the generated heat, leading to temperature increase within the cement-based composite [3]. Consequently, when the concrete mixture curing occurs in more general boundary conditions, such as pseudo-adiabatic and/or isothermal, it is necessary to adopt some advanced theoretical tools allowing the identification of the DoH. [4]. Beyond the complex problem...
characterizing the identification of the setting and hardening processes as a function of the boundary condition (i.e., adiabatic, pseudo-adiabatic and isothermal), it is worth to highlight that the early-age evolution of the cementitious composites’ properties is also governed by the intrinsic characteristics of the mixtures: cement and aggregates type and amount, possible use of alternative binders, water-to-binder ratio etc. [5][6].

As reported by Fairbairn & Azenha [7], massive structures are those structures for which the effects of cement hydration in the setting and hardening phases can cause cracks in early-age concrete mixtures. In the past, such cracking risks were considered relevant only for massive concrete structures, where the dissipation of the hydration heat was normally slow and, therefore, high temperature increases were observed. Nowadays, with the diffusion of high-performance concrete, the risk of cracking in “young” concrete is no longer a peculiarity of the massive structures. The higher quantities of cementitious materials associated with lower water-to-cement ratios result, respectively, in greater heat of hydration and in microstructures with finer pores, thus generating greater amplitudes of thermal gradients and autogenous shrinkage [7]. For this reason, giving the definition of massive structure, it was done in a broad sense, considering all the concrete elements for which the effects of the hydration of the cement can involve risks of thermal cracking. A very significant case, reported by Betioli et al. [8] concerns the hydroelectric dam of Itaipú (located on the Paraná river, on the border between Paraguay and Brazil) whose construction began in 1975. During its the construction, cracking phenomena were observed. At that time, as reported by Rosso & Piasentin [9], the analyzes indicated that this crack pattern was due to the heat of hydration observed in the field, which was considerably greater than that assumed during the dam project. It was also found that the models to simulate the behavior of early-age concrete were very simplified and did not took into account the stress concentrations induced by the elements’ geometry. To improve the dam behavior, various measures were taken such as changing the mix design of the concrete or introducing additional reinforcements in some areas. In addition, existing cracks were injected with epoxy and corresponding structures examined by an intensive monitoring program. Another relevant example concerns a dam built on the Blue River, in China, inaugurated in 2006. For this demanding work, as reported by Zhang et al. [10], a first report on concrete mix design was developed in 1998, in which some problems were highlighted. They mainly concerned the need to obtain, on the one hand, a concrete with high mechanical strength, so as to cope with the dynamic impacts due to the dragging of stone materials into the watercourse. On the other hand, the produced mixtures should have been able to have a structure as free as possible of cracks of thermal origin which may have been linked to an excessive dosage of cement required to achieve high mechanical strength. The results obtained in this first phase of the study were satisfactory for the mechanical strength required and for the associated resistance to erosion, but not acceptable for the high cracking state recorded on the surface of the first castings, due to the tensile stresses induced by the excessive heating in the central core of the structures and stresses induced by the hygrometric shrinkage of the concrete surface. Therefore, it was decided, in 2001, to perform new research to reduce the cracking, exploiting the possible use of different raw materials and various mixture proportioning.

In this context, this paper presents a detailed description of a numerical procedure which is capable of simulating the time evolution of a concrete’s early age temperature development under semi adiabatic conditions [11][12]. In this numerical procedure the differential heat equation takes into account the heat that liberates to the environment through the formwork or concrete’s surface. This is done by considering the well-known Arrhenius Principle [13] and assuming a pre-defined shape of the adiabatic hydration curve of the concrete mixture. An iterative procedure is developed with the aim to bring the simulated temperature development (which depends on both the assumed adiabatic curve and the thermal boundary conditions) to match the actual temperature measurements recorded in a sample of concrete during setting and hardening stages. This modelling/identification procedure, enabling various boundary conditions, ranging from semi-adiabatic to isothermal, can be employed to simulate the time evolution of the DoH of a concrete strucuture.
2. Theoretical formulation

2.1. Fundamental assumptions of a theoretical model for cement hydration

The hydration reaction which develops in concrete mixture can be analysed by means of a theoretical approach recently proposed in the literature by the authors of this paper [11]. As a matter of fact, the proposed modelling approach is able to assess and simulate the time development of the degree of hydration (DoH, identified with the symbol \( \alpha_h(t) \)). The latter, in fact, is identified by the ratio among the heat \( Q(t) \) which is produced up to a certain time \( t \) and the maximum heat \( Q_{\text{max}} \) which can be potentially produced as a result of the whole cement reaction:

\[
\alpha_h(t) = \frac{Q(t)}{Q_{\text{max}}} \quad (1)
\]

As a consequence, the reaction of the cement results to occur in a heat transfer process and, consequently, in a transient temperature field \( T \) which can be described by the following equation describes the \( T \) field when it develops in a 1D domain (see also the schematic representation proposed in Figure 1):

\[
\rho_c c_c \frac{\partial T}{\partial t} = \lambda_c \frac{\partial^2 T}{\partial x^2} + q_c(x,t) \quad , \quad (2)
\]

In the above-mentioned equation (2), the term:
- \( \rho_c \) represents the is mass per unit volume of the produced mixtures;
- \( c_c \) is the specific heat of the concrete mixtures;
- \( \lambda_c \) represents the thermal conductivity coefficient and;
- \( q_c(x,t) \) is the rate of heat production of concrete.

Moreover, the “heat production of concrete” \( (q_c(x,t)) \) is defined as follows:

\[
q_c(x,t) = C \frac{2Q}{\partial t} \quad . \quad (3)
\]

The analytical equations presented by equation (3) and, then, \( Q(x,t) \) cannot directly evaluated since they depend on the actual temperature which is developed within the concrete mixture sample.

On the other hand, the following equation (w) describes the cement heat production (labelled as \( Q_a(t) \)) for the case in which the concrete sample is cured in adiabatic boundary conditions: [13]:

\[
Q_a(t) = Q_{a,\text{max}} e^{-\tau^\frac{t}{\nu}} \quad . \quad (4)
\]

where:
the term $Q_{a,max}$ (which is minor than the $Q_{max}$) represents the actual amount of heat produced at the end of the reaction (in adiabatic conditions);

- $\tau$ and $\beta$ are two numerical parameters controlling the shape of the adiabatic curve.

Therefore, the rate of the produced heat $q_a(t)$ is defined by introducing the expression proposed by equation (4) within the rate definition defined by equation (3). However, the heat concrete production ($q_c(x,t)$) is not generally equal to the $q_a(t)$ occurring in adiabatic condition. This is due to the fact the different temperatures develop inside the concrete sample cured in different boundary conditions (i.e., adiabatic and non-adiabatic). Despite this, based on the well-know Arrhenius Principle [13], it is possible to correlate the $q_c(x,t)$ and $q_a(t)$ where the former can be expressed in terms of the later and substituted in eq. (2). As a consequence, the numerical problem turns into an integral-differential equation [11]. To solve it, initial and boundary conditions should be defined:

$$T(x,t=0) = T_R$$

in which the term “$T_R$” represents the initial room temperature.

On the other hand, the boundary condition are defined by the characteristics of the border between the cured concrete mixtures and the surrounding external condition. For instance, when semi- (or pseudo-) adiabatic conditions occur, the following relationship can be defined in order to guarantee the continuity of heat flow throughout the insulating layer and the external environment:

$$
\frac{\lambda_p}{t_p} \frac{T_{\text{left}}(t) - T_R}{T_{\text{right}}(t) - T_R} = \lambda_c \frac{\partial T}{\partial x}_{x=-L/2}, \frac{\lambda_p}{t_p} \frac{T_{\text{left}}(t) - T_R}{T_{\text{right}}(t) - T_R} = \lambda_c \frac{\partial T}{\partial x}_{x=L/2}.
$$

in which:

- $L$ represents the specimen’s length in the $x$ direction (heat flow direction);
- $t_p$ is the thickness of the insulating layer;
- $\lambda_p$ represents the thermal conductivity of the insulating layer.

It is worth to mention that, in the case in which the concrete mixture is cured under isothermal conditions and at a constant (in time) room temperature ($T_R$) the following boundary conditions can be defined:

$$T(x = -L/2, t) = T_R, T(x = L/2, t) = T_R.$$

2.2. Indirect identification of hydration reaction processes

The proposed modelling approach presented in the in the previous section, leading to the resolution of the integral-partial-differential problem (defined by equation (2)) once the boundary conditions are defined (see equation (6) and/or (7)) can be easily employed for simulating the time evolution of the temperature ($T$) occurring within the curing concrete sample. This simulation can be symbolically denoted by the following equation (8):

$$T_{th} = T_{th}(x,t;q_r, q_f),$$

where the vectors $q_r$ and $q_f$ include the two following sets of parameters:

$$q_r = \left[ T_R, Q_{max}, \alpha_{h,max} \right], q_f = \left[ \tau, \beta, \lambda_p \right].$$

where the components of the vector $q_r$ can be directly measurements or defined by analytical expressions already within the literature [14]. On the other hand, the components collected in $q_f$ are determined for each concrete sample by solving the following unrestrained optimisation problem:

$$\Delta(q_r, q_f) = \sum_{k=1}^{n} \left[ T_{\text{exp}}^{(k)} - T_{th}(x=0,t_k;q_r, q_f) \right]^2$$


\[ \bar{q}_f = \arg\min_q \{ \Delta(q_r, q_r') \} \].

The values obtained for each concrete mixtures (for both \( q_r \) and \( q_f \) vectors) are, then, use for simulating the actual hydration processed occurring within the concrete samples.

3. Model application

3.1. Definition of the case study

The formulated numerical procedure presented in the previous section, and recently validated in previous studies [11][12], remarks that the hydration processes as well as the time-evolution of the concrete’s mechanical performances, are governed by the composition of the cement-based mixture (identified through the parameters \( Q_{\text{max}}, q_h, \tau, \beta \) presented in section 2), the concrete element geometry (i.e., the length \( L \)) and the boundary condition both in terms of insulation characteristics (i.e., \( L_p \) and \( \lambda_p \)) and room/ambient temperature (i.e., \( T_R \)).

Once the key parameters are identified, it is possible to proposes some parametric analyses on representative mixtures considering the variation of the above-mentioned properties. In this context, the present section proposes the analysis of different concrete mixtures characterized by three different strength classes (low-strength C25/30, medium-strength C35/45 and high-strength C50/60 as defined by the Eurocode 2 [15]). The concrete mixtures are designed with the same the water-to-cement ratio, equal to 0.40, maximum size of the aggregates (equal to 16 mm) and the amount of the free water (equal to 215 l/m³) which warranty the same slump class (value ranging from 100 mm and 150 mm) for all the analysed mixtures. On the other hand, in order to reach different strength class, three different types of Portland Cement (32.5, 42.5R and 52.5R in accordance with the EN 197-1: 2011 [16]) are considered for achieving the desired characteristic strength at 28 days (i.e., \( R_{28} \)) [15]. The main characteristics of the mixtures under consideration are summarised in Table 1.

### Table 1. Properties and characteristics of the concrete mixtures considered in this study.

| Description                              | C25/30 | C35/45 | C50/60 |
|------------------------------------------|--------|--------|--------|
| Mean cylindrical compressive strength - \( f_{c,28} \) [MPa] | 34.56  | 45.35  | 57.80  |
| Characteristic cubic compressive strength - \( R_{c,28} \) [MPa] | 32.00  | 45.00  | 60.00  |
| \( Q_{\text{max}} \) [kJ/kg]             | 295    | 380    | 400    |
| Parameters defining the adiabatic temperature curve shape | \( \tau \) f | 15.0    | 12.0    | 10.0    |
|                                           | \( \beta \) | 0.80    | 0.80    | 0.80    |

Based on the numerical procedure described in section 2, it is possible to evaluate the adiabatic curve for each type of employed cements, through the calibration of the parameters \( Q_{\text{max}}, \tau \) and \( \beta \) which have been introduced defined in equation (4). It is worth to mention that these calibrations are based on the best fits of the values proposed by the Italian guidelines on structural concrete production [16]: also the results of these analysis are summarised in Table 1.

3.2. Temperature profiles and cracking risk assessment

As already mentioned, once the concrete mixture composition has been defined, it is possible to simulate the time evolution and the space development of the temperature within the curing concrete element through the numerical procedure summarised in section 2.. For instance, the following Figure 2 proposes the resulting temperature curve simulation which is obtained in the central point of a 1 m concrete element composed of high-strength concrete mixtures (i.e., C50/60 in Table 1) which has been cured either in adiabatic and isothermal (i.e., the concrete surface is not covered by any isolating layer and the ambient temperature presents a constant value equal to 20 °C) conditions. The proposed figure highlights that, although the ambient temperature \( T_R \) is kept constant, the distribution of the
temperature in the centre of the concrete element behaves in a “quasi-adiabatic” condition: this phenomenon is associated to the element’s geometry as well as to the thermal properties of the employed cementitious mixtures. Moreover, since the temperature developments is directly associated to the time-evolution of the DoH, the latter is governed by the curing boundary conditions. This evidence is also confirmed by the curves reported in Figure 2 (e.g., see the secondary vertical axes).

**Figure 2.** Temperature and DoH development: representative numerical simulation.

The simulation proposed in Figure 2 allow to trace the temperature profiles at the early-age for concrete elements during their hydration process, as also demonstrated in Figure 3 in which this simulation is presented for 1 m and 2 m thickness element by also considering the possible variation of the concrete strength class: low strength C25/30, C35/45 and C50/60) which were produced with different types of cement and were cured in isothermal condition (\(T_R=20^\circ C\)). More specifically, the coloured maps proposed in Figure 3 show the time and space (thickness) temperature variation up to 6 curing days.
These kind of graphs (see Figure 3) give the possibility to perform an indirect verification of cracking risk phenomena which may occur in cementitious mixtures. In fact, in accordance with the Italian guidelines released by the Superior Council of Public Works [16], it is possible to prevent the cracks formation due to the thermal stresses, by avoiding that the maximum concrete temperature reaches above 70 °C and, moreover, the various part the concrete element present a gradient temperature below 20 °C. In fact, since the proposed procedure allow to predict the evolution of the temperature in curing concrete, it can be also applied for unveiling the key design parameters (e.g., element geometry and boundary condition) for mitigating the cracking risk occurring in structural concrete: for instance, by the possible application of thermal insulating moulds and/or the use of hot/cold water when the external ambient temperature is outside of the recommended range.

Finally, it is worth to highlight that, as also demonstrated in previous studies [12][18], the key output of the proposed model (i.e., degree of hydration in time) can be correlated with relevant mechanical properties of concrete (i.e., compressive and tensile strength and elastic modulus), by considering the various scenario in which the concrete elements is cured.

4. Conclusion
This study presented a theoretical modelling approach aimed at simulating the heat and the hydration processed occurring in hardening concrete and, the following main conclusions can be drawn out:
- the model furnishes a practical simulation of the time-evolution of either temperature and DoH in concrete elements cured in adiabatic, pseudo-adiabatic and isothermal boundary conditions;
- the 1D flow hypothesis turns out the model to be a useful tool for analysing the data obtained from early age concrete structures and, moreover, it can be easily used for the assessment of the cracking phenomena due to thermal stresses occurring in hardening concrete;
- one of the next step of the present research is the possible correlation of the key output model (i.e., DoH development) with the corresponding concrete mechanical properties. This, will allow to propose a more advanced simulation tool for the verification of the thermal cracking risk;
- consequently, the system proposed herein can be also used as a practical tool for construction site monitoring of temperature rise and forecast removal of formworks.

Figure 3. Temperatures development in (a) 1 m and (b) 2 m early-age concrete (adapted from [18]).
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