Modeling of Stress Distribution During Portland Cement Curing in Temperature Gradient Conditions

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Abstract. The paper presents the two-dimensional model of Portland cement curing based on the finite element method. The cement curing lasts for 2 days in the temperature gradient conditions ranging from 65 to –20 °C. A cement rod 7×70 cm in size was used for modeling the von Mises stress distribution. It is shown that in the temperature gradient conditions, the stress maximum in curing Portland cement shifts toward the hot edge of the cement rod and exceeds the minimum stress level more than two times. The stress growth at the interfaces between the concrete timber and the cement rod exceeds the stress maximum inside the latter. This stress distribution is connected with the heat flow generation and superposition of direct and reverse heat flows. Superposition of the negative heat flows generates the stresses at the interfaces, which are higher than those generated by the positive heat flows. The concrete timber and the interface fixation are the additional factors that increase the stress level at the interfaces and promote the cement fracture.

1. Introduction
A consistent description of the cement curing process requires the quantitative data on the initial phase composition, water-cement ratio, activation energy of the dissolution of clinker phases, heat generation in forming the intermediate and final products, porosity, bound moisture, ion composition of aqueous solution, humidity, external conditions, and elastic properties of hydration products. The experimental study of cement curing based on a set of variables of this multi-component system is rather difficult. It is necessary to create the model for the cement curing. The Virtual Cement and Concrete Testing Laboratory (VCCTL) [1, 2] allows evaluating the content of the main hydration products and strength gain during the curing process. But the VCCTL modeling of Portland cement curing is performed in isothermal conditions. The investigation of the strength gain characteristics of curing Portland cement at an early stage involves the heat and mass transfer, the evolution of physical and mechanical properties of the material with variable composition. The methods of description of heterogeneous temperature fields and hydration mechanisms of Portland cement allow to predict the evolution of mechanical properties of the materials in a wide temperature range and in the temperature gradient conditions. This approach provides a complex representation of the dependence between the material properties and the main variable parameters for the process control at different curing stages. Temperature gradients result from an exothermic chemical reaction between water and a cementitious binder. Model-based testing of Portland cement properties as a binder significantly reduce the time, materials and human resources in determining its physicochemical properties after 28 days of curing.
This work focuses on the numerical simulation of the cement curing mechanism at the initial stage and in temperature gradient conditions. The investigated Portland cement is similar to that manufactured at the Topki Cement Plant (the Novosibirsk region, Russia).

2. Modeling of Portland cement hydration

The curing mechanism of Portland cements in difficult conditions of heat and mass transfer can be predicted by modeling the strength gain during the operation of thermal sources and mechanisms of new phase formation during the hydration process. After cement setting, the distribution of the effective heat flows induced by the external temperature gradients and thermal sources, can be considered in the approximation of a homogeneous medium and, as a consequence, the evolution of the heat and mass transfer – within the diffusion mechanisms. According to Neville [3], the linear expansion coefficient, which refers to the main parameters of the cement paste, varies between $11 \times 10^{-6}$ and $20 \times 10^{-6}$ K$^{-1}$. Thermal expansion of cement is affected by temperature, humidity and its phase composition. Temperature also affects the elastic moduli. At the initial stage, Portland cement curing relates to the multiphysics problem of interconnection between heat flows and strength gain during the hydration process [3]. Assuming that at the initial stage of curing, the heat redistribution in Portland cement is determined by thermal conductivity, the governing is the equation with a volumetric thermal source:

$$C_p \rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}[k(T) \frac{\partial T}{\partial x}] + \frac{\partial q(t)}{\partial t},$$

where $C_p$ is the specific heat capacity, $\rho$ is the density, $k(T)$ is the thermal conductivity coefficient, $q$ is the thermal source, which is the time and space function.

The thermal conductivity coefficient depends on the moisture content and temperature [3–5]. Here, we assume that this coefficient is constant without reducing significantly the accuracy of calculations. The main thermal sources include chemical reactions during cement setting and curing, that occur owing to hydration processes on cement grains. The hydration reaction is exothermic and leads to a noticeable heat generation. In the proposed model, the water diffusion through the hydrate layer is the dominant mechanism that determines the hydration kinetics. In the framework of the diffusion processes, the hydration products resulting from chemical reactions and mass transfer in cements can be described by the degree of hydration $\alpha(t)$, which is associated with the hydrated cement imbalance in real time $t$, and is a measure of heat released during hydration. It is assumed that the mass transfer provides the optimum dissipation of excess heat. The imbalance of free and bound moisture in hydrates is the driving force of hydration product growth [4]. With increasing temperature, the process of binding free water is enhanced by thermal activation. Since the affinity for the formation of hydrates is the driving force of hydration product growth [4], the hydration degree can be written as [6, 7]:

$$\alpha(t) = \frac{q(t)}{Q_{\text{max}}},$$

where $Q_{\text{max}}$ is the internal latent heat resulting from complete hydration, $q(t)$ is the thermal source in real time $t$.

The hydration kinetics is associated with the diffusion of free water through hydrates in the product layers surrounding the grain nuclei. During hydration, the hydrate layer increases and affects the moisture diffusion rate. The hydration degree is proportional to the normalized affinity and the temperature factor, which are taken into consideration in the Arrhenius relation. Cervera, et al. [4] propose the analytical expression for the hydration degree:

$$\frac{\partial \alpha(t)}{\partial t} = A_c(\alpha) \beta(\phi) \exp(-E_c/RT),$$

where $A_c(\alpha)$ is the normalized affinity. The temperature factor depends on the activation energy $E_c$ and temperature $T$; $R$ is the gas constant; $\beta$ is the empiric function of moisture $\phi$ [8], which can be obtained from

$$\beta(\phi) = [1 + \alpha_c(1-\phi)^k]^{-1},$$
The approximating parameters $\alpha$ and $\beta$ are 5.5 and 4, respectively [9, 10]. The analytical equation of affinity is proposed in [3, 4]:

$$A_2(a) = A_{z2}(A_{z2}/\alpha^x + a)(\alpha^x - a)\exp(-\mu_c \alpha^x),$$

(5)

where $\mu_c$ is the viscosity, $A_{z1}$ and $A_{z2}$ are the affinity parameters equaling $1.0 \times 10^7$ and $1.0 \times 10^4 \text{ h}^{-1}$, respectively [10]; $\alpha^x$ is the asymptotic hydration [4, 5]. The latter can be found from

$$\alpha^x = (1.031\,\omega) / (0.19 + \omega),$$

(6)

where $\omega$ is the water-cement ratio. Hydration as a measure of heat releasing during the hydration process in real time $t$ is connected with the internal thermal source (1). After this,

$$q(t) = \rho Q_{\text{max}} \frac{d\alpha(t)}{dt},$$

(7)

Based on the experimental data, another approximating functions are given in works [11–13]. They allow evaluating the heat generation in real time $t$ during hydration. In particular, for adiabatic conditions,

$$q(t) = Q_{\text{max}} (1 - \exp(-rt)), \quad q(t) = Q_{\text{max}} \exp(-t/\beta^2), \quad q(t) = 1 - \exp(-\alpha (t - b)^c).$$

(8–10)

Also, based on the relative heat generation at different temperatures,

$$q(T(t)) = q_a(T(t))\exp(-\frac{T(t) - T(t)}{(RT_i T(t)) E_c}), \quad q_a(T_i) = C (\partial Q_0 / \partial t),$$

(11–12)

where $Q_0$ is the heat generation in real time $t$; $T_i$ is the temperature at which $Q_0$ is determined; $C$ is the cement concentration [12]; $r$, $t$ and $\beta$ are the approximating constants for the description of the heat generation development. The hydration degree is determined by complex hydration mechanisms, attempts to provide a universal description of hydration processes at various stages of cement curing, heat and mass transfer experiments, and the authors’ preferences. In terms of the heat and mass transfer in solid media, we determine the hydration degree as [12]:

$$\alpha(t) = A \exp(-E_a/RT) (1 - \alpha),$$

(13)

where $A = 11 \text{ s}^{-1}$, $R$ is the gas constant, $T$ is the temperature.

Thermal activation of Portland cement deformation at the initial stage of curing is described as $\partial \varepsilon / \partial t = k(T) \partial T / \partial t$. Assuming that the thermal conductivity coefficient is constant, we get $e = k(T - T_{\text{ref}})$, where $T_{\text{ref}}$ is the initial temperature of cement layering. The obtained relation can be used to detect the thermal stress from $\sigma = k(T)(E)\varepsilon$, where $E$ is the Young modulus. The function $f(E)$ regards a tensor coupling of strains and stresses. The formulated diffusion distribution of the heat flows, the temperature dependence of displacements and deformations, the hydration intensity allow us to utilize the finite element model in the estimation of thermal stresses, temperature gradients, time-dependent stresses at different stages of cement curing and in variable external conditions.

3. Results and discussion

Let us consider the two-dimensional model presented in Fig. 1 for Portland cement curing during two days. Using the finite element method (FEM) we calculate stresses in the elastic region. According to the plane view in Fig. 1, the $7 \times 70$ cm cement rod is placed in the concrete timber $2 \times 70$ cm in size. The temperature of the left and the right edges of the rod is 65 and $-20 \degree C$, respectively. It is assumed that the heat exchange is absent on the right edge, which is fixed.
Initially, the laying temperature of hydrated cement (cement+water) is $T_{\text{ini}} = 20, 12$ and 5 °C. The numerical simulation of the temperature and von Mises stress distributions are performed at the following cement parameters: 2300 kg/m$^2$ density, 1.8 V/(m×K) thermal conductivity, 880 J/(kg×K) specific heat capacity, $25\times10^6$ Pa Young modulus, $10^{-6}$ K$^{-1}$ thermal expansion coefficient, 38 kJ/mol activation energy. The concrete timber is characterized by a 532 kg/m$^2$ density, 1.8 V/(m×K) thermal conductivity, 2700 J/(kg×K) specific heat capacity, and 12.1 GPa Young modulus. The calculation results are shown in Figs 2–4.

Figure 1. Two-dimensional FEM of cement rod in concrete timber: 1 – cement rod, 2 – vertical and horizontal lines.

Figure 2. Temperature distribution in Portland cement depending on curing time of 3, 12 and 18 h: $a$ – $T_{\text{ref}} = 20$ °C; $b$ – $T_{\text{ref}} = 12$ °C; $c$ – $T_{\text{ref}} = 5$ °C.

Figure 3. Von Mises stress distribution in Portland cement depending on curing time of 3, 6, 12 and 18 h: $a$ – $T_{\text{ref}} = 20$ °C; $b$ – $T_{\text{ref}} = 12$ °C; $c$ – $T_{\text{ref}} = 5$ °C.
Figure 4. Dependences between the von Mises stress and the rod length (Fig. 1, horizontal line 1) at different time of curing within 24 hours: \( a - T_{\text{ref}} = 20 ^\circ C; \) \( b - T_{\text{ref}} = 12 ^\circ C; \) \( c - T_{\text{ref}} = 5 ^\circ C. \) Insets indicate a color time scale (days). Maximum curing time: 2 days.

According to Fig. 4, the stress distribution along the horizontal line is rather nonuniform. With increasing curing time, the stresses grow and reach the maximum at a \( \sim 10 \) cm distance, while the minimum is detected at a distance of \( \sim 39 \) cm. The distance slightly increases, when the temperature lowers. In approaching to the cold edge of the rod, the stress increases and reaches the maximum at the cement/timber interface. It is important to note that in the negative temperature range, the negative heat flows are induced by only the external temperature gradient. The hydration mechanisms do not work, and the identified stress distribution is then overestimated. The lowest stress is observed near the hot edge of the rod, which then significantly grows at the cement/timber interface. The decrease in the cement laying temperature down to \( 5 ^\circ C \) results in the positive stress increase by \( \sim 1.3 \) times. The stress distribution slightly changes during the temperature variation. Figure 5 plots the dependences between the von Mises stress and the rod length along the vertical line 2 shown in Fig. 1.

Figure 5. Dependences between the von Mises stress and the rod length (Fig. 1, vertical line 2) at different time of curing within 24 hours: \( a - T_{\text{ref}} = 20 ^\circ C; \) \( b - T_{\text{ref}} = 12 ^\circ C; \) \( c - T_{\text{ref}} = 5 ^\circ C. \)

As shown in Fig. 5, with increasing curing time, the stress also grows. The stress in the concrete timber is higher than in the cement rod. The stress distribution substantially depends on the laying temperature. Thus, at \( 5 ^\circ C, \) the stress in the timber exceeds that in the cement rod more than two times, in particular, at the cement/timber interface. According to the numerical simulation, the strength gain for 2 days in the temperature gradient conditions proves the complex nature of the heat flow generation during the curing process. Heterogeneous temperature fields induced by the external conditions, change the temperature distribution and the peak position owing to the operation of the volumetric thermal sources, and shift the stress maximum toward the hot edge of the cement rod. Negative temperatures provide the formation of zero (or close to zero) stresses in the positive temperature region of the cement rod. Therefore, thermal stress gradients generated in the cement rod can be higher than the strength of porous structure in real time \( t. \) The high level of thermal stress gradients remains constant for two days of curing. Cement/timber interfaces play a vital role in the curing mechanism of Portland cements. The intense chemical reactions cause the heat flow...
development in the cement rod. The superposition of direct and reverse heat flows occurs at the interfaces. These heat flows enable high thermal stresses in the cement rod, which either grow monotonically up to the highest values at the interfaces or abruptly grow in the concrete timber (see Fig. 5). The similar stress distribution is observed at the hot side of the rod and at the rod/timber interface. In the latter case, the stresses in the timber fixate any displacement of the cement/timber interface along the normal. In approaching to the cement/timber interface, the stress level increases. It should be however noted that the maximum stress values on the left edge are lower than on the right edge of the rod. According to Fig. 4, the temperature gradient is 0–(–20) °C at an ~14 cm distance from the cold edge. At \( T < 0 °C \), the negative heat flows at the interfaces generate stresses that are higher than the maximum stresses in the cement rod, viz. 12–14 MPa. Importantly, at the cold edge of the rod, hydration mechanisms do not work, and the stress level obtained in the model is overestimated.

Additionally, we present calculations for the stress distribution in the cement rod under the external conditions of the temperature gradient only. This is shown in Fig. 6.

**Figure 6.** Von Mises stress distribution along the cement rod without the contribution from thermal sources in curing time. The diagrams match the time \( t \) within 24 hours: \( a - T_{\text{ref}} = 20 °C \); \( b - T_{\text{ref}} = 12 °C \); \( c - T_{\text{ref}} = 5 °C \).

It is interesting, that the stress distribution in the rod with negative temperature gradient, i.e. in the region of 0–(–20) °C, increases and ranges between 7 and 11 MPa at the cement/timber interface. This effect is also conditioned by the superposition of the negative heat flows produced by only the external temperature gradients.

4. Conclusions
The numerical simulation of Portland cement curing for 2 days in the temperature gradient conditions showed the complex nature of the temperature and von Mises stress distribution. Nonmonotonic stress distribution along the cement rod significantly depended on the curing time, cement laying temperature, and temperature gradients. In the temperature gradient conditions, the von Mises stress maximum, which exceeded the stress minimum by 2 or 2.5 times, shifted toward positive temperatures at the rod edge. The temperature gradients promoted the formation of local stresses and minimum local stresses at the hot edge of the cement rod due to the superposition of direct and reverse thermal flows. The numerical simulation showed the complex nature of the heat flow distribution associated with exothermic reactions in the cement rod. The size of the rod and the concrete timber, and the external temperature gradients played the important role in the heat flow distribution. The reverse heat flows formed at the rod edges and the superposition of negative heat flows determined the high thermal stresses, which can go beyond the elastic regions of the cement rod which has cured for 2 days. Negative temperatures at the rod edge provided the formation of stresses in the cement rod, which monotonically increased from minimum to maximum values at the cement/timber interface due to the negative flow superposition. At the rod edge with negative temperature, the stress exceeded the maximum value of the cement rod. The level of stresses was also affected by the external fixation of the rod edge.
5. Acknowledgement
This work was financially supported by Grant №18-08-01025 from the Russian Foundation for Basic Research.

6. References
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