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Thermomechanical analysis of early age concrete by computer modeling

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Abstract. This study describes a procedure for the analysis of concrete structures where thermal properties are investigated in a finite element model to predict the temperature and stress profile elements due to the hydration process at early ages. An exponential function is used to determine the degree of hydration of the concrete; the temperature-dependent thermo-physical parameters are considered, and the external heat loss by convection. The commercial software ABAQUS was used to carry out the study and FORTRAN subroutines were developed to allow solution-dependent material properties in the calculation of thermal stress (taking into account the rising of Young's modulus). The main data are obtained from the literature and adjusted for this specific study, to predict the evolution of temperature and the tensile tendency of a concrete structure in the initial hours. The numerical results obtained in this work are well correlated with the literature values. The results show the thermal-stress behavior of a concrete block during the early age, taking into account the variation of elasticity modulus and also the weather conditions of Curitiba.

Keywords: Early-age Concrete, Hydration Degree, Mass Concrete, Thermal Stresses, ABAQUS.

1 Introduction

The chemical reaction of cement with water is an exothermal reaction that releases a large amount of heat. The heat generated is often called the heat of hydration and depends on the chemical composition and the amount of cement, Leon and Chen [1]. In massive structures, the combination of heat produced by cement hydration and relatively low heat dissipation (due to the low thermal conductivity of concrete) produces rising in concrete temperature a few days after concreting (Mehta and Monteiro [2]). Exposed surfaces, temperatures are relatively lower due to heat loss for cooling from the external environment due to convection. This phenomenon causes thermal gradients within the structure, which can lead to high tensile stresses on concrete surfaces and produce surface cracks mainly in the early ages, when the tensile strength is low (Lin and Chen [3][4]).

Preventing concrete cracking is essential to ensure its quality. The most common thermal concrete practice is to limit the temperature differential between the center and the surface of concrete structures [3], however, the temperature differential is not conclusive enough to determine the risk of cracking due to thermal stresses. Lawrence et al. [5] evaluated concrete block bridges and reported that the temperature differential alone was not sufficient to determine the thermal stresses. Silvoso [6] shows that the initial temperature of the concrete influences the adiabatic elevation of the concrete since the reaction is thermoactivated. Nagy and Thelandersson [7] and Chen and Lin [4] pointed out that the development of Young's modulus of concrete is very important in the modeling of thermal stresses. Do et al [8] suggested the importance of tensile strength development and creep behavior in tensile stresses.

During the hydration process of early age concrete, both thermally induced stresses and concrete strength are developing, but at different rates [4], and cracking tends to occur at locations where the tensile stress exceeds the tensile strength. In practice, this cracking time is most likely to occur within 1 to 2 days after concreting, depending on element geometry, size, boundary conditions, mix concrete, curing conditions, concreting temperature and ambient temperature variations (Tia et al [9] and Mehta and Monteiro [2]).

Due to the complexity of the non-uniform thermal loading of the heat of hydration, as well as the non-uniform temperature-dependent properties of the concrete material at an early age, numerical approaches such as the finite element method using commercial software such as ABAQUS, ANSYS, and DIANA have been widely used. applied for thermomechanical analysis of mass concrete at early ages (Do [10], Yikici, Sezer and Chen [11], Leon and Chen [12], Amin et al [13], Sargam et al. [14], Teixeira [15]] and Coelho [16]).

In this study, the thermal properties in the early age of mass concrete are investigated based on the work of Lin and Chen [3] and [4] and adapted to the weather conditions of Curitiba-PR, Brazil. Then, with the thermal analysis performed, the temperature predictions are used in stress analysis, considering the constant and variable elastic modulus in the initial hours. The temperature results obtained were compared with the values of the literature and the results of stress obtained were compared with the tensile strength of the concrete to verify its structural integrity.

2 Thermomechanical analysis: material properties

The governing equation for a solid 3D heat transfer problem is presented in eq. (1), where $\mathrm{T}, \mathrm{t}, \mathrm{K}_c, \rho, \mathrm{C_p}$ and q are temperature (°C), time, thermal conductivity (J/mh°C), density (kg/m³), specific heat (J/kg°C), and heat generation rate (J/m°C), respectively, and x, y and z are the coordinates (m). The equation considers the orthotropic behavior of the material, with the thermal conductivity varying according to the orientation, however, in this study the simplified model will be used, which considers the isotropic behavior of the thermal conductivity, that is, without variation of the values as a function of the direction.

$$\frac{1}{\rho C_p}\left[\frac{\partial}{\partial x}\left(K_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial T}{\partial z}\right)\right] + \frac{q}{\rho C_p} = \frac{\partial T}{\partial t} \tag{1}$$

The thermal analysis for concrete becomes complex since the thermal conductivity, specific heat and the rate of heat generation depend on the maturity of the concrete [1]. Thus, in the first stage of the development of this study, the aim is to validate the model created using commercial software ABAQUS, according to the results presented by Lin and Chen [3], who performed a thermal analysis of the first ages in a concrete block. Thus, the geometric characteristics of the analyzed concrete block [1.2m x 1.2m x 1.2m], as well as the characteristics of the concrete mix and chemical composition can be seen in Lin and Chen [3].

To calculate the thermally induced stresses, it is necessary to estimate the tensile strength of concrete and the development of the elastic modulus over time [4]. The properties vary as a function of temperature and time, which determines the degree of hydration of the concrete (Yikici, Sezer and Chen [11]). The degree of hydration $\propto (te)$is calculated using eq. (2), used to estimate the strength and elastic modulus of concrete at a given time, is a function of the equivalent age, te. The equivalent age can be calculated using the Arrhenius equation, eq. (3) [17], which depends on the activation energy E_a; from the concrete temperature history $T_c(t)$, which is obtained from the experimental studies by Lin and Chen [3] by extracting points from the temperature curve and creating a seventh-order approximation to obtain an equivalent equation via software MAPLE; and the final degree of hydration $\propto_u$, eq. (4) proposed by Mills [18]. Then, the rate of heat generation at any equivalent age $q(t)$ can be determined by eq. (5).

$$\propto (\mathrm{te}) = \propto_{\mathrm{u}} \exp\left(-\left(\frac{\tau}{\mathrm{te}}\right)^{\beta}\right) \tag{2}$$

$$\mathrm{te} = \int_0^{\mathrm{t}} \exp\left(\frac{\mathrm{E_a}}{\mathrm{R}}\left(\frac{1}{\mathrm{T_r}} - \frac{1}{\mathrm{T_c(t)}+273}\right)\right) \mathrm{dt} \tag{3}$$

$$\propto_u = \frac{1.031\frac{w}{c}}{0.194\frac{w}{c}} \tag{4}$$

$$\mathrm{q(t)} = \mathrm{Q_c} \propto (\mathrm{te}) \left(\frac{\tau}{te}\right)^{\beta} \frac{\beta}{te} \exp\left(\frac{\mathrm{E_a}}{\mathrm{R}}\left(\frac{1}{\mathrm{T_r}} - \frac{1}{\mathrm{T_c(t)}+273}\right)\right) \tag{5}$$

Where E_a: activation energy equal to41841 J/mol as determined by Yikici and Chen [19] following the procedures of ASTM C 1074 [20]; R: universal gas constant 8,314 J/mol°C; $T_c(t)$: temperature of the concrete in time (°C); T_r: reference temperature (296K); w/c: water-cement ratio of concrete; β and τ hydration parameters that control the shape of the hydration degree curve, with values of 0.94 and 14, respectively [3]; and $\mathrm{Q_c}$ is the total heat available equal to 1.67x10^8 J/m³ mixture, determined as a function of the total cement content in the concrete (kg/m³) and the total hydration energy per kilogram of cement (J/kg) obtained using Bogue's calculation [21].

With the determination of the degree of hydration of the concrete $\propto(te)$ and the equivalent time te, it is possible to calculate the concrete properties that vary over time, that are: thermal conductivity K_c and specific heat C_p; and the mechanical properties: compressive strength f_c', tensile strength f_{ct}, and modulus of elasticity E_c.

The thermal conductivity K_c (J/mh°C) of the concrete reduces over time, being able to present a decrease of 33% during the hydration process and can be calculated by eq. (6), as proposed by Van Breugel [22]. The specific heat of concrete C_p (J/kg°C) depends on the proportions of the concrete mix, degree of hydration, and the temperature of the concrete, according to eq. (7).

$$K_c(\propto_r) = K_{uc}\big(1.33 - 0.33 \propto_r (t)\big) \tag{6}$$

$$C_p\big(\propto_r, T(t)\big) = \frac{1}{\rho}\big(W_c \propto_r C_{cef} + W_c\,(1 - \propto_r)C_{cem} + W_s C_s + W_a C_a + W_w C_w\big) \tag{7}$$

Where: K_{uc}: is 1.87 W/mK; $\propto_r(t) = \propto(te)/\propto_u$; ρ: is the density of the mass of the concrete per unit of volume, being 2400 kg/m³; W_c: the mass of cement per unit of volume is 335 kg/m³; W_s: the mass of fine aggregate per unit of volume is 844 kg/m³; W_a: the mass of aggregate per unit of volume is 969 kg/m³; W_w: the mass of water per unit of volume is 139 kg/m³; C_{cem}: specific heat of cement at 740 J/kg°C; C_s: specific heat of the fine aggregate at 710 J/kg°C; C_a: the specific heat added at 840 J/kg°C; C_w: the specific heat of water at 4184 J/kg°C; C_{cef}: fictitious specific heat of the hydrating cement given by eq. (8) (J/kg°C).

$$C_{cef} = 8.4\,(T_c(t) + 273) + 339) \tag{8}$$

For the thermal analysis, the heat transfer between the solid element and the fluid by convection is considered using Newton's law of cooling (Burmeister [23], Abeka et al. [24]). In this study, based on Lin and Chen [3], free convection with a value of 7.9 W/m²K is adopted as the free convection coefficient for the interface between the concrete surface and the air.

The mechanical properties of the concrete are taken into account over time as a function of the degree of hydration of the concrete. Several studies present the compressive strengths f_c' and tensile strengths f_{ct} (MPa) as a function of the degree of hydration of the concrete, according to eq. (9) and eq. (10), respectively (Lin and Chen [4], Do et al [8], Schutter [25], Frølich et al [26]).

$$\mathrm{f}_c' = 45.53 \propto (te) - 1.71 \qquad (\propto(te) \geq 0.04,\ \mathrm{f}_c' \geq 0) \tag{9}$$

$$f_{ct} = 0.53\sqrt{45.53 \propto (te) - 1.71} \qquad (\propto(te) \geq 0.04,\ \mathrm{f_{ct}} \geq 0) \tag{10}$$

The elastic modulus E_c (MPa) is determined by eq. (11) based on tests performed by Lin and Chen [3], where it is assumed that Young's modulus develops as a function of the hydration degree and presents the same value in the tensile and compression directions. The elastic modulus increases the strength of concrete and directly influences the determination of thermomechanical stresses (Neville [27]), and its consideration in the analysis is important.

$$E_c = 5407(45.53 \propto (te) - 1.71)^{0.492} \quad (\propto(te) \geq 0.04,\ \mathrm{E_c} \geq 0) \tag{11}$$

With the determination of the thermomechanical properties of the concrete, the modeling, analysis, and obtaining of the results begin.

3 Simulation process and results

The analyzes of the concrete element at early ages were implemented using the commercial software ABAQUS and contained two steps successive: thermal analysis and stress analysis. The time-temperature history, material properties, and analysis time (120h) are based on the work of Lin and Chen [3][4]. The thermal analysis is performed in three parts: 1. 2D modeling for model validation compared with the results obtained by Lin and Chen [3]; 2. Adaptation of the 2D model to local weather conditions, considering the city of Curitiba-PR, Brazil; 3. 3D modeling of the concrete block to obtain the temperature profile used in the stress analysis. The stress analysis was performed with two variations: constant elastic modulus over time and variable elastic modulus over time.

The block has dimensions of 1.2m x 1.2m x 1.2m and the following concrete properties are considered in the modeling: thermal conductivity, thermal expansion, specific heat, initial temperature and ambient temperature, Surface film condition, density, elasticity module, Poisson's ratio and generation of heat. Mechanical boundary conditions are applied to the base, constraining displacement in the block; and the thermal boundary conditions are the initial concreting temperature, the ambient temperature on the external faces of the block, and the heat generation flux of the concrete.

Taking into account the effects of material properties as dependent on age and temperature history and the non-uniform hydration process, the user-defined subroutine "USDFLD" was developed and incorporated into the finite elements. During thermal analysis, each element is treated individually for its heat generation rate [eq. (5)] and thermal properties [eq. (6) and eq. (7)] based on their degree of hydration [eq. (1)], that is, with the hydration degree updated, the thermal conductivity, specific heat, and heat generation rate are updated for the next time step; and in the stress analysis, the temperature field obtained in the thermal analysis is applied and the elastic modulus is adjusted as a function of the degree of hydration of the concrete [eq. (8)].

3.1 Thermal analysis: Model validation and adaptation to the local temperature

The validation of the model, part 01, was performed by comparing the results obtained by Lin and Chen [3] experimentally with the modeling performed via ABAQUS. The 2D model has 5250 elements and 5436 nodes using the DC2D4 element (4-node linear quadrilateral heat transfer). The temperature results in the center of the block are illustrated in Figure 1: the values obtained by Lin and Chen [3], and in the application via ABAQUS (FEM). The second part of the analysis took place after the validation of the model, that is, the results obtained in the thermal analysis of stage 01 converged with the results obtained by Lin and Chen [3]. Thus, in part 02, the model was modified to adapt to the weather characteristics of Curitiba, aiming at results more consistent with the local reality. The following changes are applied:

a) Variation of the real ambient temperature in the city of Curitiba [28]

b) Considering 120h starting on 05.24.22 - 10h until 05.29.22 - 10h.

c) Considering concreting temperature at 19 degrees.

The results obtained correspond to the expected behavior, with a reduction in the maximum temperature obtained in the block due to the initial concreting temperature and the external temperature variation. Figure 1 shows the temperature variation in the central node of the block (maximum temperature obtained) in the analysis of Part 01 and Part 02. Figure 2a illustrates the temperature profile of the block at the moment of highest temperature (18h) for the analysis of Part 01 and Figure 2b illustrates for the analysis of Part 02.

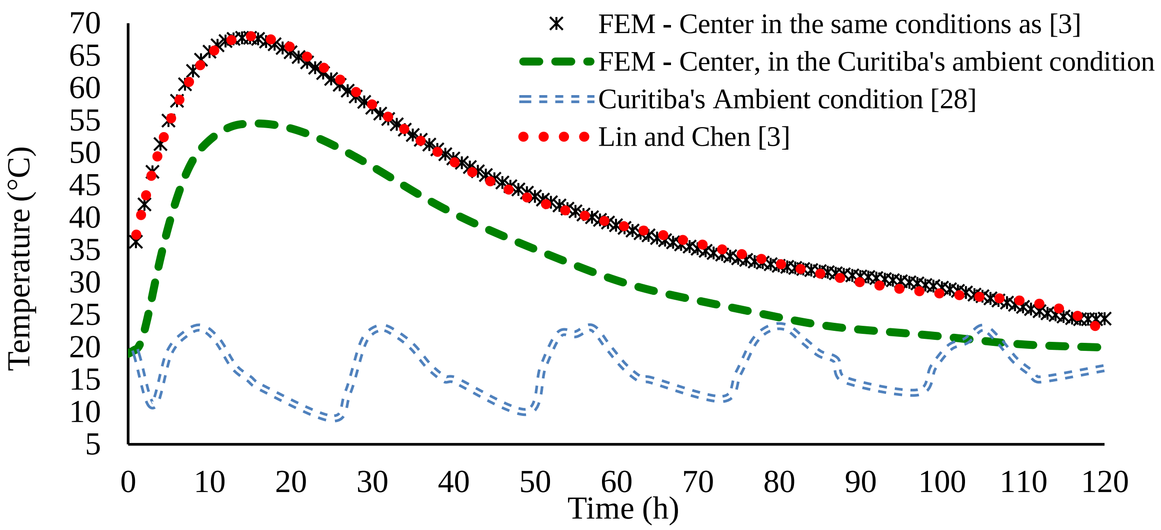

Figure 1. Center temperature of the cube and Curitiba's ambient temperature (authors and Lin and Chen [3] results)

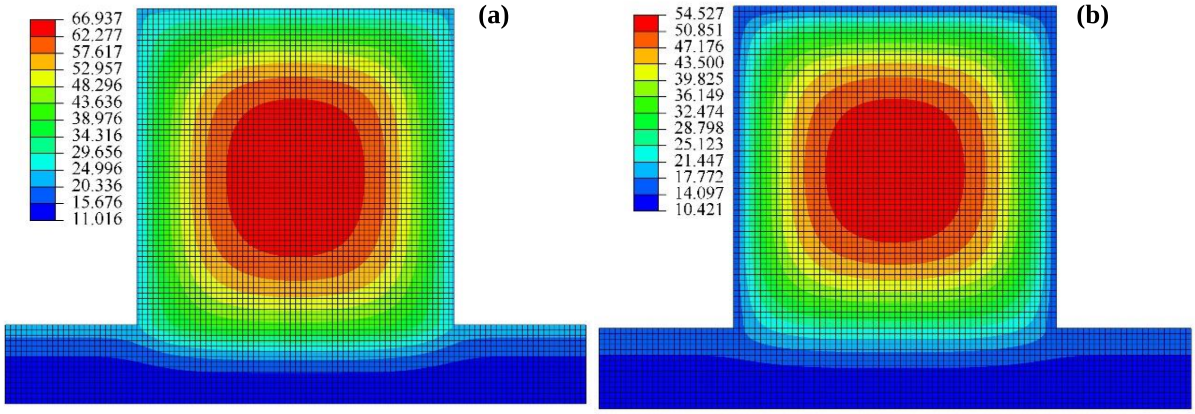

Figure 2. (a) Temperature profile analysis part 01 and (b) part 02 at 18h after casting.

The results obtained in Part 02 were saved and used in the static analysis to determine the tensile thermal stresses at the initial ages

3.2 Thermomechanical analysis: thermal stresses

Thermomechanical analysis of the concrete block was carried out to verify the stress generated due to the temperature produced in the initial hours of concreting. For this, the stress analysis was performed for the 1.2 m concrete cube using the ABAQUS program and the FORTRAN subroutine. The model has 64000 elements and 68921 nodes using the C3D8R element (8-node linear brick, reduced integration, hourglass control) with an element size of 30mm. The temperature results obtained by the "Heat Flux" analysis were coupled to the stress analysis as an input parameter for each time step.

Two analyzes were carried out to obtain the thermal stresses: the constant modulus of elasticity over time, using the value obtained by eq. [11] at the final analysis time of 120h; and with the modulus of elasticity varying over time as a function of concrete hydration, the USDFLD subroutine was defined to implement this behavior in the analysis. Poisson's ratio was considered constant in both analyzes with a value of 0.18.

Analyzes show that due to temperature evolution and thermal expansion, the internal elements were expanding resulting in surface elements in traction. The contour patterns of the stresses calculated with the constant and variable modulus are similar. For the study adapted to the weather conditions of Curitiba, the tensile strength of concrete [Eq. (10)] was not exceeded. The predicted tensile strength and the tensile stresses at critical locations for both analyzes are compared in Figure 3a and the behavior of the stress in the block is illustrated in Figure 3b at 16h after concreting, time when maximum stresses are reached.

The consideration of the constant elastic modulus results in lower tensile stresses in the initial hours than considering the elastic modulus variable in time and from 50h after concreting, the behavior of the stresses is practically identical. In both analyses, the tensile strength of the concrete is greater than the request, indicating that the material resists the efforts caused by the thermomechanical analysis and would not show cracks.

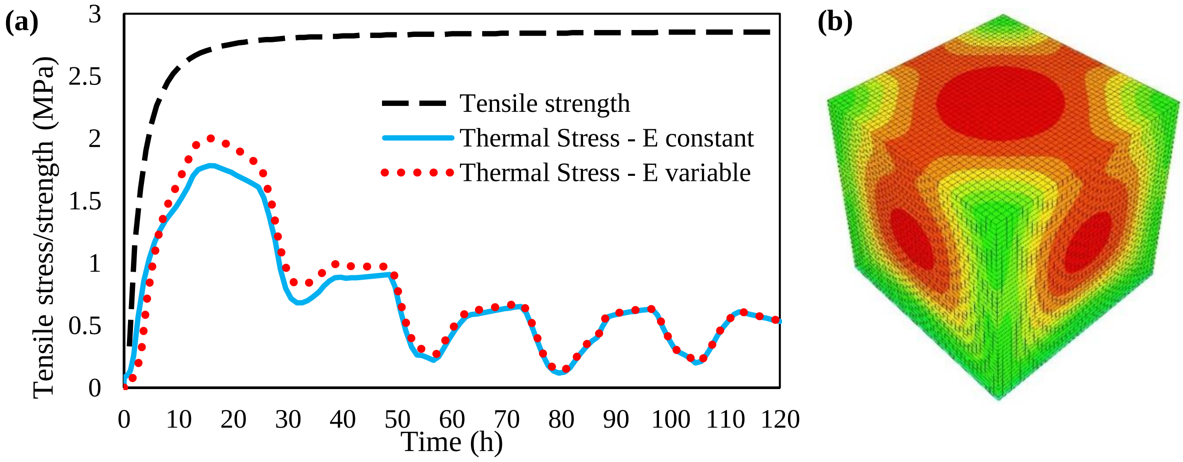

Figure 3. (a) Comparison of calculated thermal stress with constant and variable elastic model and estimated tensile strength (b) Predicted stress field of cube at 16h.

4 Conclusions

This article describes a method to perform the temperature history and thermal stress for early ages concrete using the ABAQUS program with the aid of user subroutines for 1.2m concrete cubes. The concrete temperature history and the properties of the mixture are based on Lin and Chen [3] and adapted to the weather characteristics of Curitiba-PR. Thermal properties, including specific heat, thermal conductivity, and heat generation rate, were considered dependent on the degree of hydration and determined individually for each element in the model; and in the mechanical properties, the degree of hydration is used to estimate the variation of the elastic modulus and the development of strength of the concrete. Convection on the external surface of the concrete with the environment was considered. The results show the influence of the initial concreting temperature on the heat generation of the concrete block and that the tensile stresses must be carefully predicted to avoid thermal cracking. In addition, estimating the temperature difference can allow engineers to take preventive actions to minimize the risk of thermal cracking.

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