Computational modeling for simulation of post-cooling systems in mass concrete structures

Igor A. Fraga[1], Ana B. C. G. Silva[1], Eduardo M. R. Fairbairn[1]

[1]*Programa de Engenharia Civil (PEC), Instituto Alberto Luiz Coimbra de Pós-graduação e Pesquisa de Engenharia (COPPE), Universidade Federal do Rio de Janeiro (UFRJ) Centro de Tecnologia - Av. Horácio Macedo, 2030 - Bloco I-116 - Cidade Universitária, Rio de Janeiro - RJ, 21941-450 ifraga@coc.ufrj.br, anabeatrizgonzaga@coc.ufrj.br, eduardo@coc.ufrj.br*

Abstract. Due to the high costs and safety requirements of construction and infrastructure works, thermal cracking of young concrete has been a concern of the engineering community since the first applications of mass concrete. The heat generation during hydration and the consequent increase in the temperature of the concrete are very important, not only because they can generate thermal gradients in space and time, responsible for the appearance of high initial stresses, but also because deleterious phenomena such as the formation of delayed etringite formation (DEF) have been shown to be associated with the existence of thermal fields in the early ages of cementitious material.

In this way, this work will present the numerical implementation for simulating a post-cooling model for mass concrete structures, on a mesoscopic scale, in which the temperature of the material is reduced during hydration by the circulation of water in tubes embedded in the forms by a post-cooling system. The implementation was executed using the finite element method (FEM), in a parallel computing environment, coupled to the TENCIM software, developed in FORTRAN programming language, developed by PEC / COPPE / UFRJ.

Keywords: post-cooling, numerical formulation, mass concrete, cooling tube

1 Introduction

According to RILEM [1], “mass concrete structures are structures in which the hydration effects of cementitious materials at early ages, such as heat generation and autogenous shrinkage, can lead to cracking”.

As the hydration reaction is exothermic and the thermal conductivity of concrete is relatively low, it usually endures temperature rises that are especially relevant in massive concrete structures. Two types of relevant thermal gradients can be identified in mass concrete: (i) one is relative to time, that is, a given point of the structure has its temperature varying over time; (ii) another is a spatial gradient that corresponds to the temperature difference, at a given instant, between two different points of the structure. Considering the thermal expansion of concrete and the structural restraints to free deformations, both gradients mentioned above can be responsible for the generation and evolution of strain and stresses in the concrete elements. If such strains or stresses reach a certain limit, undesirable thermal cracks can occur.

The generation of heat and the consequent rise in the temperature of concrete are very important, not only because they can generate thermal gradients in space and time, but also because deleterious phenomena such as the Delayed Ettringite Formation (DEF) have been prove to be associated with the existence of fields thermals in the early ages that reach temperatures of the order of *65 ºC*. The set of issues mentioned adequately supports the claim that the increase in temperature due to hydration is a very important issue with regard to the durability of the structure.

Therefore, the construction phase and subsequent period must be accurately analyzed. If the tendency to cracking is detected, many actions can be taken to minimize early stresses, such as: (i) decreasing the construction speed, allowing higher heat dispersion; (ii) reducing the placement temperature of the concrete; (iii) decreasing the concrete temperature by circulating water or air in tubes embedded in the formwork (post-cooling systems); and (iv) choosing a material composition that gives lower heat of hydration rates.

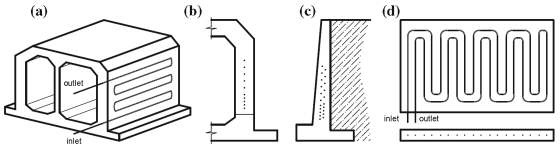

Figure 1. Examples of structures with post-cooling systems.

Due to the high costs and safety requirements of construction and infrastructure works, thermal cracking of young concrete has been a concern of the engineering community since the first applications of massive concrete. The evolution of knowledge on the subject led to the development of theories that consider the hydration reaction as exothermic and thermally activated. Such theories led to sophisticated numerical models that, together with the evolution of hardware and software, allowed the development of very complex simulation models that approached reality in terms of geometry and phenomenological models considered [2].

This work will present the results of the implementation of a concrete post-cooling simulation model, developed by Fraga et al. [3], on a mesoscopic scale, in which the temperature of the concrete during hydration is reduced by the circulation of water or air in tubes embedded in the formwork. The model was implemented and coupled in the finite element program TENCIM, developed in FORTRAN programming language and parallel environment, by PEC/COPPE/UFRJ.

2 Post-cooling systems

Post-cooling of concrete with embedded tubes (*post-cooling*) has been applied since the 1930's [4]. The objective is to control the internal temperature of the concrete within the limits specified in the project through the active circulation of water (or other cooling fluid) or air through the tubes embedded in the material, to mitigate the risk of the appearance of cracks of thermal origin. It is generally oriented towards reducing peak concrete temperatures during the hydration period, thus minimizing the volumetric variations associated with the corresponding temperature variations. The design of post-cooling systems comprises the optimization of tube properties (geometric layout, heat transfer, fluid flow, inlet/outlet temperatures) to achieve the desired peak temperature reduction with the least possible energy consumption .

Examples of structures and their corresponding typical tube layouts can be seen in Fig. 1 [5]. The technique is quite effective, but it has considerable design, material acquisition, installation, and effective operation costs. For this reason, its general application area is limited to larger ones, such as dams that mold internal cooling before filling/ sealing the joint [6]; the cooling system can be activated in the first days after concreting, allowing thermal control of the concrete. Other post-cooling applications include, but are not limited to, production of concrete segments for immersed tunnels, retaining walls and slabs [7] [8] [9], which are commonly used today Made and using dedicated finite element analysis (FEA) software.

3 Numerical modeling of the post-cooling system

3.1 Formulation

In most practical applications, the flow of a fluid through a pipe or duct can be approximated to be one-dimensional, and thus the properties can be assumed to vary in one direction only (the direction of flow). As a result, all properties are uniform at any cross section normal to the flow direction, and the properties are assumed to have bulk average values over the cross section.

The fluid velocity in a tube changes from zero at the surface because of the no-slip condition, to a maximum at the tube center. Therefore, it is convenient in this work a mean velocity υ_w, which remains constant for incompressible flow when the cross sectional area of the tube is constant. The mean velocity in actual heating and cooling applications may change somewhat because of the changes in density with temperature. But, in this work, the fluid properties at some average temperature are treat as constants, as shown in Fig. 2.

The value of the mean velocity υ_w in a tube is determined from the requirement that the conservation of mass principle be satisfied. That is,

$$\dot{m} = \rho \upsilon_w A_w \tag{1}$$

where $\dot{m}$ is the mass flow rate, ρ the density of the fluid and A_w is the cross sectional area.

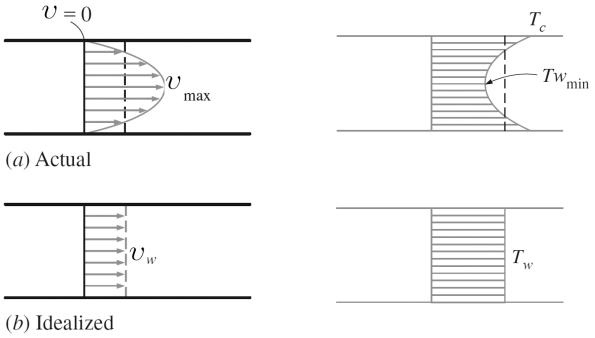

Figure 2. Actual and idealized velocity and temperature for flow in a tube. (Adapted from CENGEL [10])

When the fluid is heated as it flows through a tube, the temperature of the fluid at any cross section changes from T_c at the surface of the concrete to some minimum at the tube center. In this work is convenient a mean temperature T_w that remains uniform at a cross section. The mean temperature will change in the flow direction whenever the fluid is heated and its value is determined from the requirement that the conservation of energy principle be satisfied. That is, the energy transported by the fluid through a cross section ($\dot{E}_w$)in actual flow must be equal to the energy that would be transported through the same cross section if the fluid were at a constant temperature T_w. This can be expressed mathematically as

$$\dot{E}_w = \dot{m} C_p T_w = \int_{\dot{m}} C_p T \delta \dot{m} = \int_{A_c} \rho C_p T \upsilon dA_w \tag{2}$$

where C_p is the specific heat of the fluid.

The conservation of energy for the steady flow of a fluid in a tube can be expressed as:

$$\dot{Q} = \dot{m} C (T_w^i - T_w^0) \tag{3}$$

where T_w^i and T_w^0 are the mean fluid temperatures at the exit and inlet of the tube, respectively, and $\dot{Q}$ is the rate of heat transfer to the fluid.

The thermal conditions at the surface was approximated to be constant surface heat flux ($\dot{q} = constant$) as shown in Fig. 3. Surface heat flux is expressed by Newton's law of cooling as

$$\dot{q} = h(T_c - T_w) \tag{4}$$

where h is the local transfer coefficient.

Knowing that the mean fluid temperature increases linearly in the flow direction in the case of constant surface heat flux ($\dot{q} = constant$), and the surface area increases linearly in the flow direction (A_s is equal to the perimeter, which is constant, times the tube length), the rate of heat transfer can also be expressed as

$$\dot{Q} = \dot{q} A_s = \dot{m} C_p (T_w^i - T_w^0) \tag{5}$$

Considering that h and thus $T_c - T_w$ are constant, as the fluid properties remain constant during flow, the slope of the mean fluid temperature T_w can be determined by applying the steady-flow energy balance to a tube slice of thickness dx shown in Fig. 3. It gives

$$\dot{m} C_p dT_w = \dot{q} P dx \rightarrow \frac{dT_w}{dx} = \frac{\dot{q} P}{\dot{m} C_p} = constant \tag{6}$$

where P is the perimeter of the tube.

Then the mean fluid temperature at the tube exit becomes

$$T_w^i = T_w^0 + \frac{\dot{q} P l}{\dot{m} C_p} \tag{7}$$

where l is the lenght of the section of the tube.

Combining Eq. 1, 4 and 7 gives

$$T_w^i = T_w^0 + \frac{h(T_c^0 - T_w^0) P l}{\rho \upsilon_w A_w C_p} \tag{8}$$

$$\dot{q} = -\frac{\rho \upsilon_w A_w C_p (T_w^i - T_w^0)}{P l} \tag{9}$$

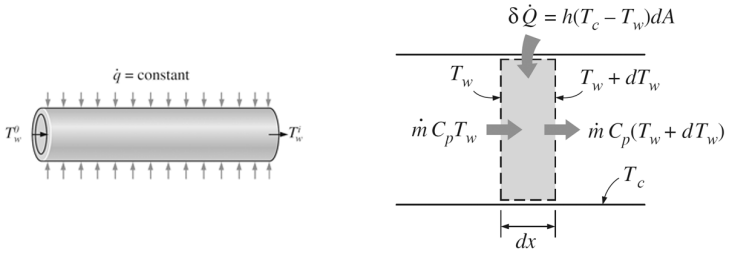

Figure 3. Tube schematic and energy interactions for a differential control volume in a tube. (Adapted from CENGEL [10])

3.2 Computational Modeling

Applying the theoretical formulation to the implementation of a numerical solution for the post-cooling of concrete structures, an arbitrary volume was considered, as shown in Fig. 4, consisting of two distinct materials: concrete and fluid.

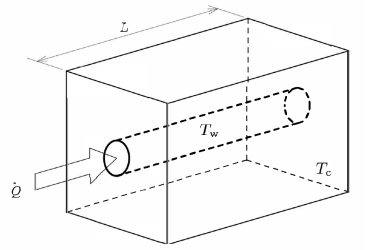

Figure 4. Concrete and fluid volume model.

Initially is considered this volume as a single isolated element, in order to simplify the fluid-solid interaction, we can define through Eq.8 and 9 the outlet temperature T_w^i of the fluid, as well as the heat flow generated by this heat exchange.

Time t_0 is considered the instant that the fluid enters in the element, and t_i the instant the fluid exits the element, determined as a function of the fluid velocity and the length of the tube section. The δt is characterized by the exchange time between both materials, defined by the lenght of stay of a given fluid control volume inside the solid, according to Eq. 10 and Fig. 5.

$$\delta t = t_i - t_o = \frac{l}{v} \tag{10}$$

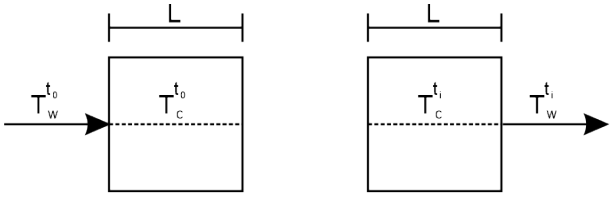

Figure 5. Temperatures at the instant t_0 and t_i.

Assuming $\dot{m} = \rho v_w A_w = \rho\dot{V} = \rho\frac{V}{\delta t}$, where V is the fluid volume, is obtained:

$$T_w^i = T_w^0 + \frac{h(T_c^0 - T_w^0)Pl}{\rho V C_p}\delta t \tag{11}$$

$$\dot{q} = -\frac{\rho V C_p(T_w^i - T_w^0)}{Pl\delta t} \tag{12}$$

Finally, the heat flow generated is distributed in the volume of the element and is added as a new heat source to the thermochemical coupling of the program, as shown in Eq. 13.

$$Q = -\rho V C_p (T_w^i - T_w^0) \tag{13}$$

In order to implement the model in the finite element program TENCIM, the representation and application of the tube mesh is by interconnected hexahedral elements, coupled to the mass concrete structe mesh geometry, and each element will represent a control volume. Thus, to simulate the fluid flow along the pipe, the fluid inlet temperature in a given element will always be given by the outlet temperature of the previous element, according to Eq. 14 and Fig. 6.

$$T_{w_n}^0 = T_{w_{n-1}}^i \tag{14}$$

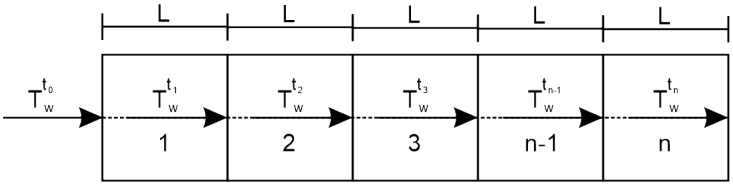

Figure 6. n elements.

Considering that the initial temperatures at time t_0 will be prescribed for both materials, and that the fluid inlet temperature in the first element $T_{w_1}^0$ will always be constant, for each time step δt a new exit temperature is calculated for each $T_{w_n}^i$ element and a heat source in the Q_n element.

4 Numerical modeling of mass concrete

The numerical model used in this work is based on the theory of thermochemical and mechanical coupling proposed by Ulm and Coussy [11] in which the equations that govern the problem are deduced within the thermodynamic theoretical framework for porous media and consider the cross-effects between the hydration reaction, temperature evolution, deformations and changes in concrete properties.

Ulm and Coussy [12] consider the concrete a chemically reactive porous medium. In its initial phase it is a fluid formed by free water and air, becoming a porous solid after reaching its percolation level.

The degree of hydration $\alpha \in [0, 1]$ is a normalized variable that expresses the evolution of the hydration reaction. It can be written as a normalization of the variable m_c that expresses the skeletal mass variation:

$$\alpha = \frac{m_c(t)}{m_{c_{t=\infty}}}, \quad \alpha \in [0, 1] \tag{15}$$

where $m_{c_{t=\infty}}$ corresponds to the solid skeleton mass formed $m_c(t)$ at time $t = \infty$ when hydration is complete.

According to the theory developed by Ulm and Coussy in their studies ([11]; [12]; [13]), given a mass of concrete, the description of the evolution of the hydration reaction is given, in order to consider the exotherm and thermoactivation of the reaction, from the solution of the equation of evolution of the thermal fields in a given volume. Thus, the equation of heat over time, considering the thermochemical coupling (hydration heat generation with thermoactivation) following the theoretical framework of thermochemical couplings, can be placed in the form:

$$C_{pc}\dot{T} = \dot{Q} + L\dot{\alpha} + \lambda \nabla^2 T \tag{16}$$

where C_{pc} is the specific heat of concrete, $\dot{Q}$ the flow of heat originating from some heat source (e.g. post-cooling system), λ is the thermal conductivity, L is a material constant, positive because of the exothermic nature of the reaction and $\dot{\alpha}$ is the reaction speed represented by the speed that the degree of hydration increases (derived from m_α with respect to time).

The term corresponding to the thermochemical coupling is $L\dot{\alpha}$ which represents the generation of heat by the hydration reaction, that is, the exotherm.

The initial fields are given by:

$$T(x, t_0) = T_0 \quad \text{em} \quad \Omega \tag{17}$$

And the boundary conditions are:

$$T = \bar{T}(\Gamma_T, t) \quad \text{em} \quad \Gamma_T \tag{18}$$

$$\mathbf{q}.\mathbf{N} = \bar{q}(\Gamma_q, t) \quad \text{em} \quad \Gamma_q \tag{19}$$

$$\mathbf{q}.\mathbf{N} = h_{pr}.(T - T_{amb}) \quad \text{em} \quad \Gamma_{C,R} \tag{20}$$

where $\bar{q}(\Gamma_q, t)$ is the flow in the Γ_q part of the contour, $\bar{T}(\Gamma_T, t)$ is the temperature prescribed in Γ_T, a Eq. 20 represents the heat exchange by convection and radiation at the boundaries of the continuum with the environment considering an average exchange coefficient (h_{pr}), $\Gamma = \Gamma_T \; cup \Gamma_q \cup \Gamma_{C,R}$ and $\mathbf{N}$ is the normal outside the boundary.

Through the Eq. 16 it is possible to calculate the temperature field as a function of the heat generated, represented by the term $L\dot{\alpha}$.

It is also noted that to find the numerical solution of the Eq.16 it is necessary to calculate the hydration field, that is, it is necessary to know α for all time steps that you want to obtain the field of temperatures T. Thus, it is concluded that to solve the Eq. 16, it is necessary to first determine the hydration kinetics $(\dot{\alpha}(\alpha))$ for each time step.

Considering then the kinetics of this hydration reaction in an integrated way, through the basic model for cementitious materials, in a law like *Arrhenius*, it is writed the Eq. 21 proposed by Ulm and Coussy [11], Ulm and Coussy [12], Ulm and Coussy [13], as the equation for the evolution of the cement skeleton mass, measured by the variation of the degree of hydration with time.

$$\dot{\alpha} = \frac{d\alpha}{dt} = \tilde{A}(\alpha) \exp\left(-\frac{E_a}{RT}\right), \tag{21}$$

where $\tilde{A}(\alpha)$ is called normalized affinity and encompasses the physical effects corresponding to the increase in hydrate mass, diffusion, viscosity and the chemical affinity itself. This is the only property of concrete that is independent of temperature.

The thermoactivation effect is represented in the equation by the exponential factor as a function of temperature, $\exp\left(-\frac{E_a}{RT}\right)$, explaining that the reaction intensifies when temperatures are higher. The terms E_a, R and T are defined as the activation energy, universal constant of perfect gases and temperature, respectively. It should be noted that in this model E_a is considered constant over time.

Thus, it is evident that if there is knowledge of a curve $\tilde{A}(\alpha)\; x\; \alpha$, it will be possible to solve the Eq. 16, as long as there is, for each time step, in addition to the temperatures T, the degrees of hydration α.

The values of $\tilde{A}(\alpha)$, which are an intrinsic measure of the reaction kinetics, can be obtained experimentally, through adiabatic tests or through uniaxial compression isothermal tests performed at different ages.

5 Application

The example adopted for the application of the computational model was constituted by an adiabatic concrete bulk, cooled by water through a tube inserted in the axis of that volume, composed of a single volume, representing the tube and the fluid, as shown in Fig. 8 and properties listed in the Tab. 1 and Fig. 7.

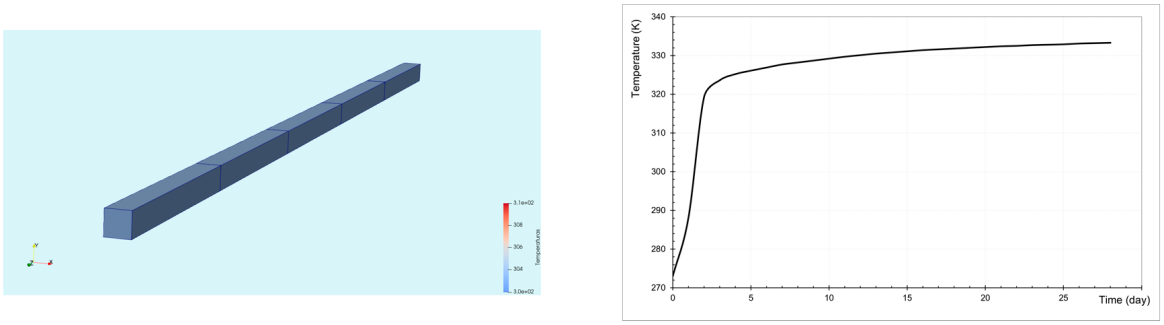

Figure 7. Finite element mesh (t=0) and adiabatic temperature rise.

The mesh is defined by 5 hexahedral elements, as shown in Fig. 7 with the first conditions of the concrete $T^0_{c_1} = T^0_{c_n} = 303K$. The adiabatic temperature rise is shown in Fig. 7. The inlet cooling water temperature is constant $T^0_{w_1} = 283K$ throughout the entire simulation.

Table 1. Material properties: concrete and coolant (water).

	Concreto	Tube + coolant (water)
$L\ (m)$	10	
$L'\ (m)$	2	
$a\ (m)$	0,2	
$b\ (m)$	0,2	
$\delta t\ (s)$	2	
$m\ (kg/m^3)$	2430	1000
$C_p\ (J/kg.K)$	908	4184
$\lambda\ (W/m.K)$	1,52	0,61
$v_w\ (m/s)$	-	1
$\phi\ (m)$	-	0,09
$h\ (W/m^2.K)$	-	60
$Ea/R\ (K)$	4000	-

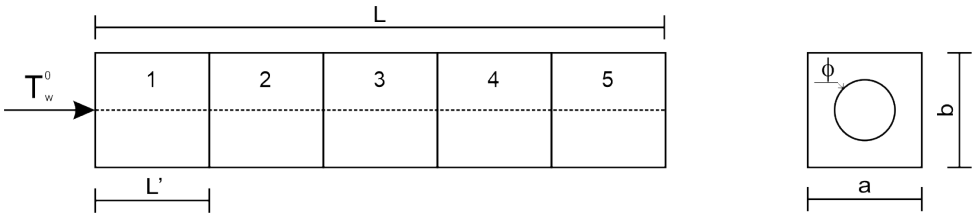

Figure 8. Example - Longitudinal and Transverse views

In order to validate the model and verify the obtained results, the same conditions of the problem were simulated in the commercial finite element software *DIANA FEA*.

The Fig. 9 presents the temperature results obtained by the proposed model, compared with the temperature data obtained by *DIANA FEA* in the volume of output element for both materials: concrete and coolant (tube + water). It is possible to verify that both results show similar behavior.

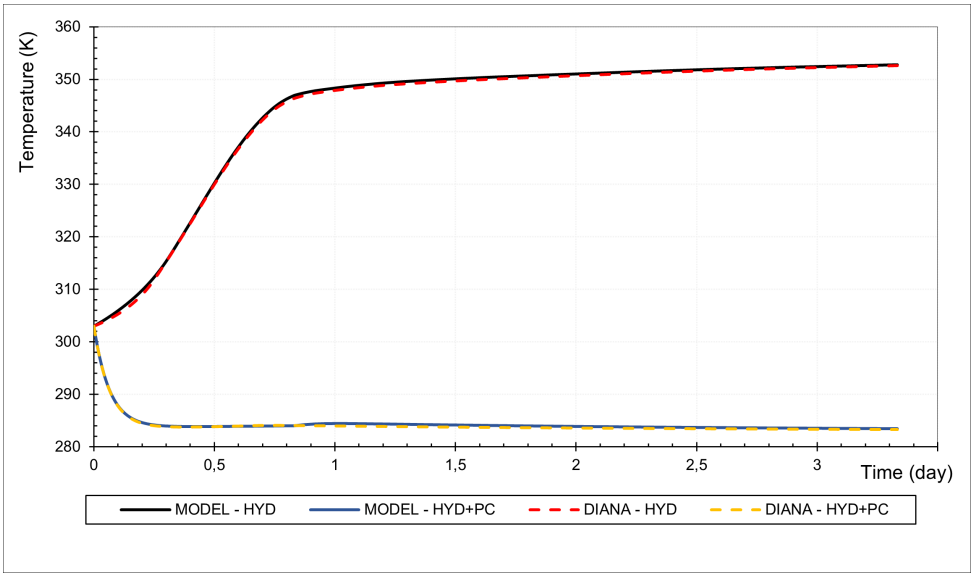

Figure 9. Result of the temperatures obtained for the last element of the model x Diana FEA (nel = 5) for concrete and coolant.

6 Conclusion

The temperature results obtained by the proposed model, compared with the temperature data obtained by *DIANA FEA* for both materials, show similar behavior, both for the hydration model without the post-cooling system, as well as for the use of coolant during the hydration period.

The model will allow for a significant reduction in the computational processing time of macro-scale models, thus enabling the analysis of structures in less time and at a lower computational cost.

Numerical modeling of post-cooling allows significant savings in the construction of large structures. Thus, developing a predictive cracking model that incorporates concrete cooling at early ages is extremely important to minimize the appearance of stresses that exceed the resistive capacity of the element and future pathologies.

In the future, the model will be designed and tested to simulate the construction of a concrete mass structure, composed of a pillar of the Tocoma hydroelectric plant, in Venezuela, using the experimental data obtained during construction as input parameters for the program.

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