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Study of The Heat Generation Due to The Hydration of Portland Cement using $FLAC^{3D}$

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Abstract. The hydration of cement is an exothermic reaction. The cement hydration reaction is a slow and long-time reaction. The hydration process can be divided into many different physical processes, of which mechanical and thermal processes are considered the most common. The analysis of temperature fields and thermal stresses in concrete structures is highly significant for preventing concrete from cracking. This paper presents the numerical simulation by using $FLAC^{3D}$ for hydration process in the concrete structures which includes heat hydration generation, heat propagation in concrete. it is possible to predict and control the amout of heat generated and their distribution in the concrete structures. In addition, it can be evaluated the dangerous level of the thermal stress and thermal deformation. These results can help the designer proposed the appropriate method for a construction process and concrete curing to achieve the best concrete quality according to the standard.

INTRODUCTION

The hydration of cement in concrete is a slow and often long-time chemical reaction. This shows that the compressive strength of concrete increases gradually over time. However, the rate of increase in strength of concrete slows down later on. According to the many research results (Phung 2006, Mafalda et al. 2013, Rajczakowska et al. 2019, Kiernozycki and Blyszko 2021) showed that the cement content in unhydrated concrete after 28 days is about 20% of the total cement. The hydration process of cement is an exothermic reaction mainly due to the hydration of C3A and C3S. There is a large amount of heat is generated during the concrete hardening due to the hydration of the cement. This is causing the temperature in the concrete to increase. Due to the poor thermal conductivity of concrete, the heat generated is concentrated in the center of concrete mass and causing the temperature difference between inside and outside of concrete mass. Over time, the temperature in the concrete will gradually decrease to an environment temperature. The process of generating heat when cement hydration causes thermal stress, which is one of the causes of cracks in concrete and reducing the lifetime of structures (Ho and Vu 2012).

The formation and distribution of heat fields in concrete depends mainly on factors such as number of aggregate particles, aggregate particles shape, cement type, content of cement, thermal properties of the aggregate materials, shape and size of structure, concrete mix, concrete curing method, environment around the structure, etc. In the civil engineering field, there are many structures with very large volume such as transfer beams, building foundations, machine foundations, dams, etc. The amount of heat of cement hydration is very large with these structures.

This paper presents the results of research on heat generation and heat transfer when hydrated cement by using $FLAC^{3D}$ program (Itasca). The simulation process is carried out in the following steps: heat generation and heat transfer by thermal models, hardening and strength development of concrete by mechanical models.

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THERMAL HYDRATION MODEL

The hydration grade is defined as the ratio between the accumulated hydration heat up to the current time (Q $[J/m^3]$) and the ultimate hydration heat generated until total completion (Q_{max} $[J/m^3]$) as following (Onken and Rostásy 1995):

$$\alpha(t_e) = \frac{Q(t_e)}{Q_{max}} \tag{1}$$

where $t_e[s]$is the concrete age.

The hydration time of cement depends on the temperature of the concrete. Therefore, the heat flow above the boundaries and the heat conductivity within the hydrating material are of specific importance for the heat transfer process. Lower temperatures of an environment lead to a longer hydration process with lower hydration heat generation, whereas higher temperatures lead to a shorter hydration process with higher hydration heat generation. The age of concrete is determined as follows:

$$t_e = \int_0^t e^{\frac{E_A}{R}\left(\frac{1}{T_{Ref}}-\frac{1}{T}\right)} dt \tag{2}$$

where: R is the universal gas constant ($R = 8.314\, J/K/mol$); E_A is the activation energy $[J/mol]$; T_{Ref} is the reference temperature which is set to 20ºC (Onken and Rostásy 1995) and T is the material's temperature.

The amount of heat generated during the hydration of cement in concrete is determined as follows:

$$Q(t_e) = C.Q_{Ce}(t_e) \tag{3}$$

$$Q_{max} = C.Q_{Ce,max} \tag{4}$$

where: C is the content of cement material $[kg/m^3]$; Q_{Ce} is the amount of hydration heat generated by the hydration process up to the current time $[J/kg]$; $Q_{Ce,max}$ is the ultimate hydration heat generated until total completion $[J/kg]$.

With respect to equations (1), (3) and (4), the current heat release is

$$q(t_e) = \dot{Q}(t_e) = \dot{\alpha}.C.Q_{Ce,max} \tag{5}$$

Without any restriction, the hydration process would run over the full range of the hydration grade, which is $\alpha = [0, 1]$. The heat release is always active, and at the end, a heat in the amount of Q_{max} has been generated. However, this process can be restricted by physical or numerical reasons. Therefore, two independent limitations are available, one depending on temperature and the other on hydration grade as follows:

$$q(t_e) = \begin{cases} q(t_e) & T \leq T_{max,q} \\ 0 & T \geq T_{max,q} \end{cases} \tag{6}$$

$$q(t_e) = \begin{cases} q(t_e) & \alpha \leq \alpha_{max,q} \\ 0 & \alpha \geq \alpha_{max,q} \end{cases} \tag{7}$$

The behavior of hydration grade depending on equivalent age in equation (2) is exponential description with the two Jonasson material parameters b $[-]$ and $t_1[1/s]$ as follows:

$$\alpha(t_e) = e^{-\left(ln\left(1+\frac{t_e}{t_1}\right)\right)^b} \tag{8}$$

The equivalent age of concrete is given in equation (2). Where the only material parameter of equivalent age is the activation energy E_A. The activation energy E_A is a function of temperature as follows:

$$E_A(T) = \begin{cases} E_{A,1} + dE_{A,T}.\left(T_{0,EA} - T\right) & T \le T_{0,EA} \\ E_{A,1} & T \ge T_{0,EA} \end{cases} \tag{9}$$

where typical parameters are: $E_{A,1} = 30\ kJ/mol$; $dE_{A,T} = 1.47\ kJ/mol/K$; $T_{0,EA} = 293\ K$;

The heat transfer is assumed to be isotropic, with the following functions of specific heat (c_p) and thermal conductivity (λ) as follows:

$$c_p = c_{p,1}.\left(1 + dc_{p,\alpha}.\alpha\right)\left(1 + dc_{p,T}.T\right) \tag{10}$$

$$\lambda = \lambda_1.(1 + d\lambda_\alpha.\alpha)(1 + d\lambda_T.T) \tag{11}$$

FLAC^{3D} MODEL FOR HYDARION PROCESS

The mechanical aspects of hydration in FLAC^{3D} are handed by a modified Drucker - Prager constitutive model where elastic and strength properties depend on the hydration grade α (Hinze 1987). This is taken into account by the minimum degree of hydration (α_o). When the hydration grade exceeds the value (α_o), the strength and stiffness of the concrete are no longer linearly dependent on the hydration grade. Then the elastic modulus of concrete during hydration process is determined as follows:

$$E(\alpha) = E_{cte}.\left(\frac{\alpha-\alpha_o}{1-\alpha_o}\right)^a \tag{12}$$

where: E_{cte} is Young's modulus after complete hydration, and a is the power exponent.

The actual uniaxial compressive strength (σ_c) and the uniaxial tensile strength (σ_t) of concrete also depend on the function of hydration rate and is determined as follows:

$$\sigma_c(\alpha) = 0{,}85.\left(\frac{f_{cte}}{c}.\frac{\alpha-\alpha_o}{1-\alpha_o}\right)^{3/2} \tag{13}$$

$$\sigma_t(\alpha) = f_{cte}.\left(\frac{\alpha-\alpha_o}{1-\alpha_o}\right) \tag{14}$$

where: f_{cte} is the uniaxial strength after total completion of the hydration process and c is a material parameter.

The yield criterion in the Drucker - Prager constitutive model is as following:

$$\tau + q.\sigma - k = 0 \tag{15}$$

where q and k are material parameters; τ and σ are stress invariants; q and k can be derived from the actual uniaxial compressive and tensile strengths σ_c and σ_t as follows:

$$q = \frac{\sqrt{3}(\sigma_c - \sigma_t)}{\sigma_c + \sigma_t} \tag{16}$$

$$k = \frac{2\sigma_c\ \sigma_t}{\sqrt{3}(\sigma_c + \sigma_t)} \tag{17}$$

SIMULATION MODEL OF HEAT GENERATION OF CONCRETE

This example consists of a concrete inclusion inside an elastic and thermal isotropic material. The model has a size of 11m × 1m × 11m as illustrated on the Fig. 1. The large concrete mass has a size of 3m × 1m × 3m. There are 5 points with coordinates of 1(5; 5), 2(4; 5), 3(3; 5), 4(2; 5) and 5(1; 5) respectively for observation of heat generation and transfer as showing in Fig. 1. The elastic material parameters and the concrete material properties are given in the table 1 and table 2 respectively.

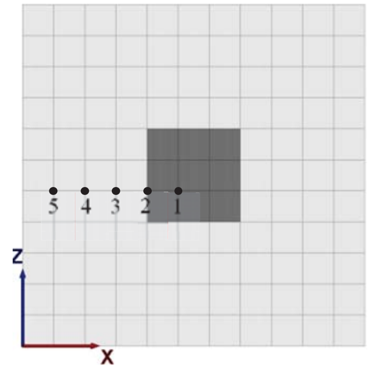

FIGURE 1. FLAC^{3D} model for the concrete inclusion test

TABLE 1. Material properties for the elastic frame

No.	Parameter	Unit	Value
1	Bulk modulus, K	MPa	1000
2	Shear modulus, G	MPa	700
3	Specific heat, C_p	J/kg/K	0.2
4	Thermal conductivity, k	W/m/K	20
5	Linear thermal expansion coefficient, α_t	$^oC^{-1}$	10^{-4}

According to the results of the researchers (Ahmadreza et al., 2015; Zainab and Hassen, 2017; Wang, 2017), the highest amount of heat is generated in the first 2 days after the concrete is placed. Therefore, the model was simulated in FLAC^{3D} by FISH routine and the heat generation and heat transfer during 2 days also simulation. The contour of temperature in model is shown in Fig. 2. During the hydration process, the maximum temperature is generated in the concrete mass and then transferred to the boundary. It can be seen that the highest temperature occurred at the center of concrete mass around 315^{o}K after two days' hydration process. The temperature in the center concrete mass increases by about 288^{o}K in compared to the initial environment temperature.

TABLE 2. Material properties for the concrete

No.	Parameter	Unit	Value
1	Maximum amout of generated heat, $Q_{Ce,max}$	J/kg	10^5
2	Cement concentration, C	Kg/m^3	330
3	Material parameter, b	-	-1.114
4	Material parameter, t_1	s	7.2x10^4
5	Universal gas constant, R	J/mol	8.314
6	Activation energy, $E_{A,1}$	J/mol	33.5
7	Activation energy, $dE_{A,T}$	kJ/mol/K	1.47
8	Specific heat, $C_{P,1}$	J/kg/K	0.2
9	Thermal conductivity, λ_1	W/m/K	2.0
10	Linear thermal expansion coefficient, α_t	$^oC^{-1}$	10^{-5}
11	Specific parameter for cement, α_o	-	0.2
12	Young's mudulus after complete hydration, E_{cte}	MPa	1000
13	Material parameter, c	-	0.4
14	Material parameter, a	-	0.6
15	Minimum value for (α - αo)	-	10^{-4}

The contour of principal stress in the concrete due to the heat generation is shown in Fig. 3. The comparison of Fig. 2 and Fig. 3 indicated that when the temperature in the concrete mass increases due to the hydration process, the thermal stresses are generated. The higher temperature point is corresponding the greater stress point. It can be also observed in the Fig. 3 that both compressive stress and tensile stress are occurred in the model. This is a possible cause of concrete cracking during the hardening phase.

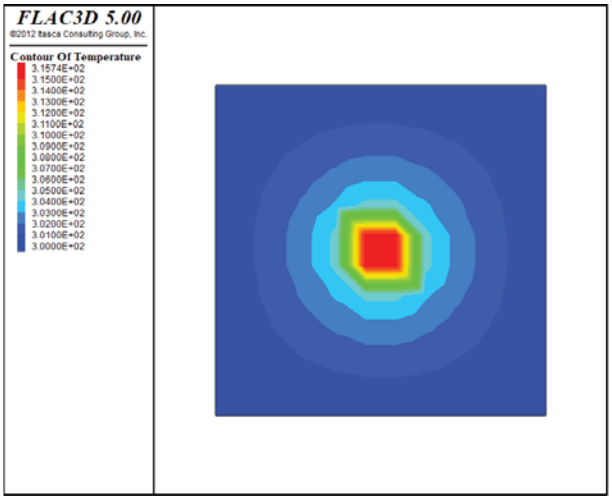

FIGURE 2. Contour of temperature in model (°K)

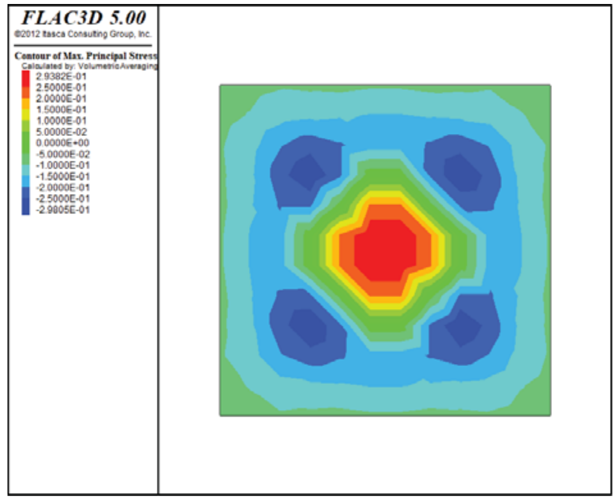

FIGURE 3. Contour of principal thermal stress

Figure 4 shows the result of temperature changes at 5 different observation points in the Fig. 1 according to the age of the concrete. It can be observed in the Fig. 4 that the heat generated by the hydration process increases rapidly from 10 to 12 hours (the end of curing process) and then decreases gradually after that (the agglomeration and strength development). At that time the maximum temperature was generated in the concrete mass and then propagation to the surrounding material mass, the temperature decreases from center to the boundary of model and close to the temperature value of the environment (300°K).

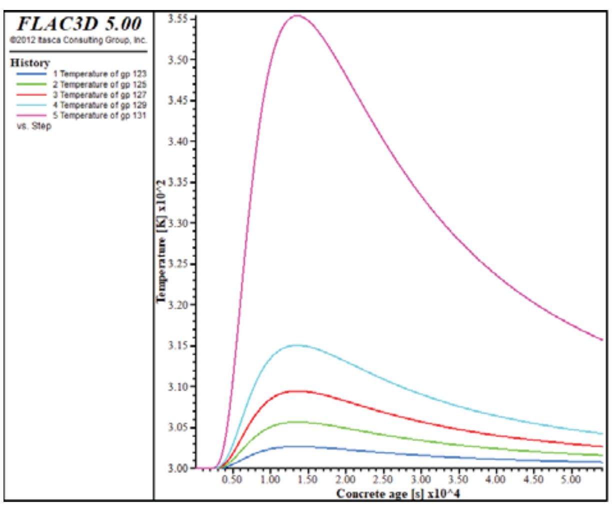

FIGURE 4. Temperature at the observation points

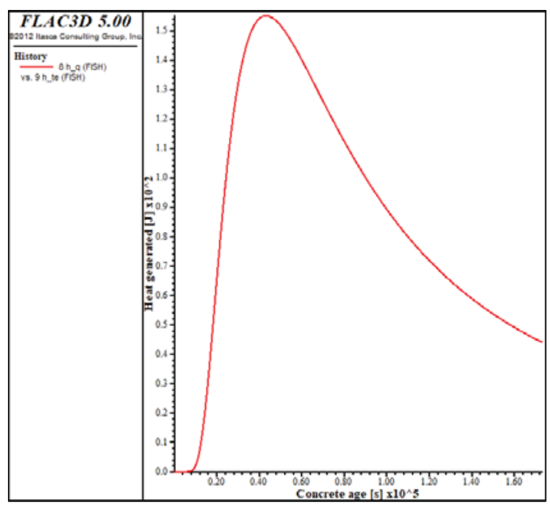

FIGURE 5. Heat generation and concrete age

The results of heat generation during hydration process are shown in the Fig. 5. It can be observed that the amount of heat generated gradually increases until about 10 to 12 hours which is the end of curing process, and then rapidly decreases with the solidification and strength development. This result is similar to the results published by Ahmadreza et al., 2015; Zainab and Hassen, 2017; Wang, 2017.

CONCLUSIONS

This paper presents the model of cement hydration, heat generation and heat transfer in concrete. The heat generated during hydration causes thermal stresses in the concrete mass and can cause cracks in the early age of concrete structures. Using the FLAC^{3D} (finite different method) to simulate the heat generation and heat transfer during the cement hydration as well as the formation of thermal stress which can decrease the quality of concrete. The simulation results indicated that the largest amout of heat is generated during the curing process of concrete, and the heat generated gradually decreases when it is transfer to the solidification and strength development stage. The strength of concrete begin to develop after a period of 18 hours and develops relatively quickly after that.

Based on the simulation results analysis, it is possible to predict and control the amout of heat generated and their distribution in the concrete structures. In addition, it can be evaluated the dangerous level of the thermal stress and thermal deformation. These results can help the designer proposed the appropriate method for a construction process and concrete curing to achieve the best concrete quality according to the standard.

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