

# Research and Application on Hydration Characteristics of Concrete Based on a Fixed Multi-field Coupling Model

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**Abstract.** Although a lot of researches about temperature-stress and crack of mass concrete have been published, there are still many work on crack control to be improved. At present, due to the development of a general chemo-thermos coupled model for hydration of concrete, multi-field coupled method has been a hot topic in the field of studying the evolution of concrete properties. Therefore, in this paper, a chemo-thermos-mechanical coupled model of concrete hydration is developed and applied to the finite element analysis. Through this method, the temperature-stress of concrete gravity dam encountering cold wave are studied. The settlement results show that this method is more consistent with engineering practice than traditional methods, and can provide reference for construction and design.

## 1. Introduction

In the field of hydraulic structure, concrete structure is a common type of long term structure selection, which accumulated abundant engineering experience during the construction of many concrete dams[1]. How to prevent the formation and development of cracks has become a key problem for dam construction and evolved as one of the hotspots in academic research[2]. There are various and complicated factors contributes the crack of the concrete dam, including material properties, environmental conditions, construction technology and quality, earthquake, cold wave and other accidental factors[3]. At different stages, there are different influencing factors, and the main causes of cracks are also different. As far as concrete cracks in high dams are concerned, they have their own characteristics. The cracks mainly occur in the early age, caused by large temperature difference between inside and outside due to the characteristics of large volume, high hydration heat, slow heat dissipation, etc[4].

On the premise of selecting suitable materials, it's extremely necessary to have a simulation for the concrete structure about its temperature-stress during its construction period. As a result, according to the simulation results, reasonable arrangement of temperature control measures can be formulated, becoming an effective way to prevent temperature cracks[5]. However, at present, most research and applications on hydration and heat release of concrete based on the linear theory, neglecting or simplifying the influence of temperature and other factors[6]. The experience of the many engineering designs has shown that, the traditional methods are prone to problems in predicting the heat release process of concrete and the development of its thermodynamic properties, easily resulting in the deviation of simulation calculation. Therefore, it is necessary to consider the effects of age and temperature simultaneously during the simulation of mass concrete component.



The heat release of concrete involves the change of energy in the chemical reaction part of hydration reaction, and the enhancement of concrete strength reflects the process of the continuous polymerization of the reactants during the chemical reaction, so the accurate prediction of the hydration heat and the strength of the concrete can be focused on the chemical reaction inside[7]. In 1998, Bentz et al.[8] gave the relationship between the final hydration degree of concrete and the water cement ratio through experiments. In 2002, Cervera et al.[9] put forward a finite element method with chemo-thermo-mechanical coupled model to proceed numerical simulation to practice concrete experiment. In 2006, Gawin et al.[10] made improvements based on previous studies, and proposed a hydration model of concrete which can be coupled with water diffusion process. In 2016, Zhou Wei et al.[11,12] modified the chemical affinity formula of the concrete hydration model considering the chemo-thermo-mechanical effect, and studied the applicability of the super sulphate cement in the mass concrete. For a further research on concrete, in this paper, a fixed formula of degree of hydration is presented. Based on the improved formula, the temperature process of concrete and the evolution process of its material properties are simulated by the chemo-thermo-mechanical multi-field coupled model. Through the simulation calculation of the engineering example, the hydration characteristics of concrete are further studied, and the feasibility of the model is verified.

## 2. Chemo-thermo-mechanical coupled model

### 2.1. A fixed model for the hydration process

A lot of research show that various physical changes in the process of hydration of concrete are mostly derived from its internal chemical reactions, which enlightened us take degree of hydration as an intermediate variable to describe heat release and properties evolution of concrete in the process of hydration. The degree of hydration can be described by the following formula:

$$\zeta(t) = \frac{m(t)}{m_{\infty}} \quad (1)$$

Where  $\zeta(t)$  is the degree of hydration at time  $t$ ,  $m_{\infty}$  is the final mass of bound water under the ideal conditions assuming that free water is fully reacted in hydration reaction, and  $m(t)$  is the mass of bound water at time  $t$ .

According to Arrhenius's law, the time-dependent hydration progress could be described as in Equation (2). In the model of hydration, the relationship between hydration rate and temperature, chemical reaction affinity can be described as follows:

$$\frac{\partial \zeta}{\partial t} = A_{\zeta}(\zeta) \exp\left(-\frac{E_a}{RT}\right) \quad (2)$$

Where  $E_a$  is the activation energy of the reaction,  $R$  is a constant for ideal gases, and  $A_{\zeta}(\zeta)$  is chemical affinity at degree of hydration  $\zeta$ .

Based on the study of Cervera et al., Zhou Wei[12] has revised the expression of chemical affinity to the following forms:

$$A_{\zeta}(\zeta) = \beta_1 (\beta_2 + \beta_3 \zeta + \zeta^2) (\zeta_{\infty} - \zeta) \exp\left(-\bar{\eta} \frac{\zeta}{\zeta_{\infty}}\right) \quad (3)$$

Where  $\beta_1$ ,  $\beta_2$  and  $\beta_3$  are material coefficients,  $\zeta_{\infty}$  is the ultimate hydration degree, and  $\bar{\eta}$  represents the viscosity due to micro-diffusion of the free water through the already-formed hydrates.

### 2.2. The heat transfer process

The transient heat conduction process of concrete can be described in the following way:

$$\rho C \frac{\partial T(x, y, z, t)}{\partial t} = \lambda_T \Delta T(x, y, z, t) + \frac{\partial Q}{\partial t} \quad (4)$$

$$\frac{\partial Q}{\partial t} = Q_\infty \frac{\partial \xi}{\partial t} \quad (5)$$

Where,  $\rho$ ,  $C$ ,  $\lambda_T$ ,  $\Delta$  and  $Q_\infty$  are the density, volumetric heat capacity, thermal conductivity coefficient, Laplacian operator and the final volumetric heat of hydration, respectively.

### 2.3. Calculation of temperature-stress calculation

Under the assumption of strain superposition, the strain of concrete can be seen as following five parts: elastic strain, fracture strain, creep (or viscoelastic) strain, temperature strain and shrinkage strain:

$$\dot{\epsilon}(t) = \dot{\epsilon}_e + \dot{\epsilon}_{cr} + \dot{\epsilon}_c + \dot{\epsilon}_T + \dot{\epsilon}_{sh} \quad (6)$$

Where  $\dot{\epsilon}_e$ ,  $\dot{\epsilon}_{cr}$ ,  $\dot{\epsilon}_c$ ,  $\dot{\epsilon}_T$  and  $\dot{\epsilon}_{sh}$  are the elastic strain rate, creep strain rate, cracking strain rate, thermal strain rate and shrinkage strain rate, respectively.

Ignoring the influence of concrete creep and simplifying it, the formula of stress evolution can be obtained as follows:

$$\dot{\sigma} = E_{(\xi)} \dot{\epsilon}_e = (\dot{\epsilon} - \dot{\epsilon}_c - \dot{\epsilon}_T - \dot{\epsilon}_{sh}) \quad (7)$$

**2.3.1. Young's modulus and Poisson's Ratio.** Taking the degree of hydration  $\xi$  as an intermediate variable, the development of the elastic modulus of concrete can be described as the formula (8). According to the results of De Schutter[13], the Poisson's ratio of concrete can be estimated according to the following Equation (9).

$$E_{(\xi)} = \left( \frac{\xi - \xi_0}{1 - \xi_0} \right)^{r_e} E_\infty \quad (8)$$

$$\mu_{(\xi)} = (\mu_\infty - 0.49e^{-10}) \sin\left(\frac{\pi}{2}\xi\right) + 0.49e^{-10\xi} \quad (9)$$

Where  $E_{(\xi)}$  and  $\mu_{(\xi)}$  represent Young's modulus and Poisson's Ratio at the degree of hydration  $\xi$ ;  $E_\infty$  and  $\mu_\infty$  represent ultimate Young's modulus and ultimate Poisson's Ratio;  $\xi_0$  is the degree of hydration of concrete at the initial setting, usually been advisable to be 0.2;  $r_e$  is fitting coefficient.

**2.3.2. Thermal Strain and Shrinkage.** In general, the temperature strain of concrete is considered to be only related to temperature change, so it can be calculated by formula (10). The relevant experimental results show that there is a linear correlation between the volume deformation of concrete and the degree of hydration. Therefore, the volumetric shrinkage strain can be simulated by linear function or piecewise linear function as formula (11).

$$\dot{\epsilon}_T = \alpha_t \dot{T} \mathbf{I} \quad (10)$$

$$\dot{\epsilon}_{sh} = -(k_a \dot{\xi} + k_b) \mathbf{I} \quad (\xi > \xi_0) \quad (11)$$

Where  $\alpha_t$  is the thermal expansion coefficient, and  $\mathbf{I}$  is the unit tensor;  $k_a$  and  $k_b$  are material parameters.

## 3. Analysis of Engineering Practice

In this section, the multi-field coupled method is applied to the analysis of a roller compacted concrete gravity dam located at Yunnan, China when there is a cold wave. Compared with the conventional model, the advantages of the multi-field coupled model are briefly analysed.

### 3.1. General situation of the engineering

This project is located on the upper reaches of Lantsang River in Badi Township, Weixi County, Yunnan Province. It's total reservoir capacity is 265 million m<sup>3</sup> with the main function of power generation. Lantsang River basin is dominated by southwest monsoon climate which is distinguished as dry season and wet season. Weixi county is located on the low latitude plateau, with a long winter and without summer.

Cold wave is one of the main meteorological disasters in China, which can occur in all parts of the country, and can cause frost, freezing damage and other natural disasters. Due to its characteristic of wide range of cooling and influence, cold wave usually brings great damage to new concrete components.

### 3.2. Simulation of cold wave

Regarding the simulation of cold wave, Zhu Bofang[3] put forward a approximate formula to calculate the surface temperature of concrete during cold wave.

$$T = -f_1 A \sin \left[ \frac{\pi(\tau - \tau_1 - \Delta)}{2P} \right], \tau \geq \tau_1 \quad (12a)$$

$$\left. \begin{aligned} f_1 &= 1 / \sqrt{1 + 1.85u + 1.12u^2}, \Delta = 0.4gQ \\ P &= Q + \Delta, g = \frac{2}{\pi} \tan^{-1} \left( \frac{1}{1 + 1/u} \right) \\ u &= \frac{\lambda}{2\beta} \sqrt{\frac{\pi}{Qa}}, \beta = \frac{1}{(h/\lambda_s + 1/\beta_0)} \end{aligned} \right\} \quad (12b)$$

Where  $f_1$  is surface cooling coefficient of concrete,  $A$  is the decreasing amplitude;  $Q$  is the diachronic period of cold wave;  $\lambda$ ,  $a$  and  $c$  represent thermal conductivity, thermal diffusivity and specific heat capacity of concrete;  $\beta_0$  is the exothermic coefficient between the outer surface of the insulation board and the air;  $h$  is thickness of insulation board;  $\lambda_s$  is thermal conductivity of insulation board.

This project started construction in October 11, 2017, assuming that it suffered a cold wave in December 17, 2017. This cold wave cool 8 degrees centigrade in 3 days. The remaining boundary conditions are simulated according to actual construction conditions.

### 3.3. Finite element model

We select a slope dam section for modelling. Its finite element mesh stereogram is shown in Figure 1.

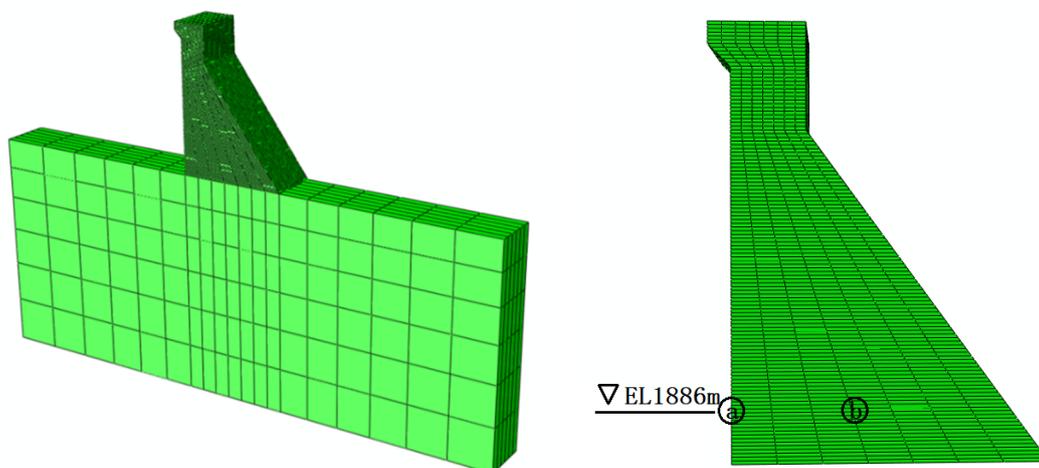


Figure 1. 3D FE mesh model of the selected slope dam section.

In the calculation of temperature, the bottom and 4 sides of the bedrock are adiabatic. The top surface exposed to the air is the third type of heat dissipating surface. The two lateral sides of dam are insulated surfaces, the other sides of dam are dissipation surfaces.

In the stress calculation, the bottom of bedrock are constrained in three directions. And the other 4 sides of the bedrock is constrained in normal direction. In the process of calculation, the gravity and temperature load of dam and bedrock are considered.

### 3.4. Parameters of concrete material

The slope dam section is mainly poured with fly ash concrete. Referring to experimental data provided by the constructor, Table 1. lists thermodynamic parameters of concrete used in the project.

Table 1. Thermodynamic parameters of concrete material.

Concrete	Density ( $kg / m^3$ )	Thermal diffusivity ( $m^2 / h$ )	Thermal conductivity ( $kJ / m^{\circ}C$ )	Specific heat ( $kJ / kg^{\circ}C$ )	Coefficient of thermal expansion ( $10^{-6} / ^{\circ}C$ )	Adiabatic temperature rise ( $^{\circ}C$ )	
						$T$	$n$
C <sub>90</sub> 20W4F50	2440	0.0030211	6.64	0.9117	5.1	14.70	2.738
C <sub>90</sub> 15W4F50	2440	0.0030604	7.08	0.9333	5.2	13.30	3.808

<sup>a</sup> The result of adiabatic temperature rise is fitted by hyperbola formula:  $T = \frac{T_0\tau}{\tau + n}$

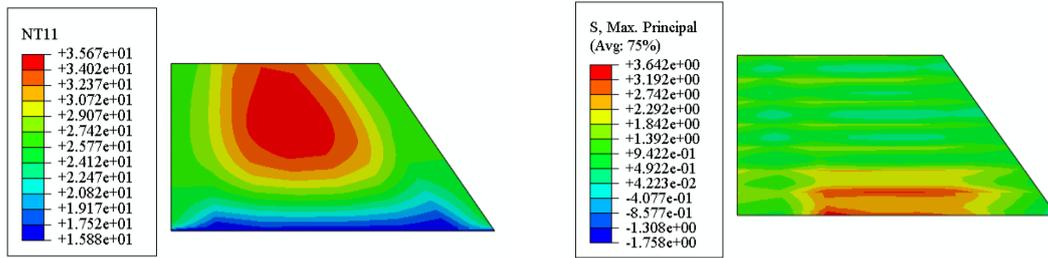
Using the approach in Section 2.1 and Section 2.2, combined with experimental data of temperature rise experiment, through the back analysis method, we get the parameters needed in the model of the degree of hydration, which are shown in Table 2.

Table 2. Parameters for the hydro-thermal model.

Concrete	$\beta_1$	$\beta_2$	$\beta_3$	$\zeta_{\infty}$	$\eta$	$Q_{\infty}$	$E_a/R$
	( $10^7h^{-1}$ )	( $10^{-4}$ )					
C <sub>90</sub> 20W4F50	6.3	9.5	-0.016	1	8.6	19200	5000
C <sub>90</sub> 15W4F50	7.4	8.2	-0.012	1	8.5	18550	5000

### 3.5. Analysis of cold wave condition

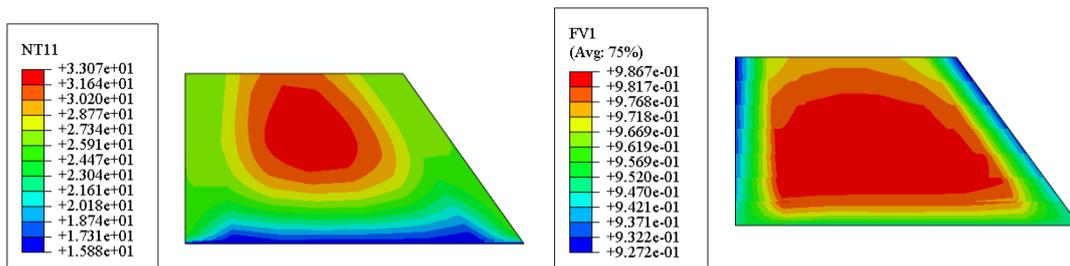
In this section, the temperature field and stress field of the slope dam section are simulated by conventional calculation method and multi-field coupled calculation method respectively. In order to make a more comprehensive analysis of effect caused by cold wave on the temperature-stress of concrete dam, the simulation results during two weeks after the cold wave are observed. Figure 2. and Figure 3. below are the results of simulation using traditional method and the results of simulation using multi-field coupled method at two weeks after encountering cold wave.



(a) Temperature field cloud picture

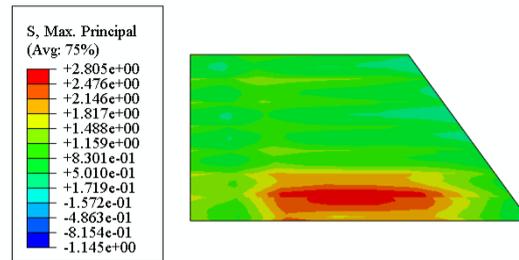
(b) Stress field cloud picture

Figure 2. Simulation results of conventional method.



(a) Temperature field cloud picture

(b) Chemical field cloud picture



(c) Stress field cloud picture

Figure 3. Simulation results of multi-field coupled method.

Comparing the results at January 1, 2018 (2 weeks after encountering cold wave) of two different methods, it can be seen that except for slightly difference in the newly poured concrete, the colour distribution of the temperature field cloud picture is basically the same, indicating that temperature field distribution of the two methods is similar. Comparing with the extreme value, it can be seen that the maximum temperature of concrete calculated by coupled method is lower than the conventional method. The upper and lower limits of the stress field calculated by the coupled method are all lower than those of the conventional method.

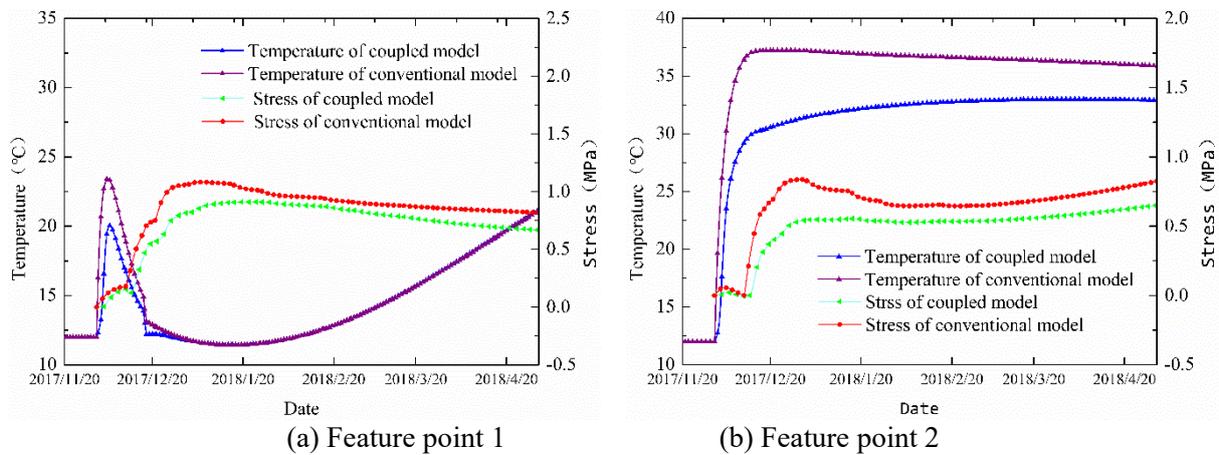


Figure 4. History curve of temperature-stress at feature point.

It can be seen from the history curve that, on December 17, 2017 the day encountering cold wave, the temperature curves of the feature points 1 on the dam surface shows a steep slope-like decline. The temperature calculated by multi-field coupled model increase more slowly in early age and get less affected by temperature change. The main reason is that, the multi-field coupled model takes the internal temperature as the reference variable for the heating reaction leading a slower heat releasing rate, which also leads a lower Young's modulus causing a smaller rise on stress after encountering cold wave.

#### 4. Conclusion

In view of the disadvantages of the conventional model on prediction of hydration heat release and properties evolution of concrete, this work introduces a fixed hydration model to describe chemo-thermo-mechanical coupled process of concrete structure, which shows a better agreement to practice. Focusing on the chemical-physical responses of mass concrete structures, a multi-field coupled method is used to analyse the temperature and stress of concrete dam encountering cold wave. The following results were obtained through this research:

A chemo-thermo-mechanical coupled model combined is introduced, which overcomes the shortcoming that conventional model only relates the heat liberation rate to time.

Taking the degree of hydration as the intermediate variable, the relation between the thermodynamic parameters of concrete and the degree of hydration is established, which is applied to a finite element calculation.

This multi-field coupled method is applied to the temperature-stress calculation of the concrete gravity dam encountering cold wave. The results show that multi-field coupled model is more consistent with engineering cognition and is of higher adaptability.

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