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Dynamic model of temperature rise caused by cementitious materials hydration

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Abstract

This paper presents a dynamic model of temperature rise caused by cementitious materials hydration based on the basic nature of chemical change. There are many models for computation of temperature rise caused by cementitious materials hydration, but the most takes this temperature rise as a function of concrete age only, which does not consider the impact of initial temperature and temperature rise during hydration and thus cannot reflect the real course of temperature rise. This model not only accords with the general law of chemical change, but also coincides well the experimental data and stimulates well the actual course of temperature rise of concrete under any initial temperature.

Keywords: Temperature; Cement; Hydration; Reaction; Dynamic model

1. Introduction

In recent years, concrete crack becomes more and more serious in concrete structure of dams, foundation works, bridges, culverts, launders and even in medium or small concrete components. Plenty of engineering survey and analysis shows the main cause of cracks is temperature rise caused by cementitious materials hydration and external temperature change [1].

The generation and development of concrete temperature and temperature stress is a complex course of chemical and physical change. The thermal variation in early stage of concrete can be described by the course of heat of hydration. The higher the temperature is, the faster the chemical change and also the quicker the concrete temperature rise during hydration. Some experiments show that when the temperature is 20, 30, 40 and 50 °C, the speed ratio of hydration is 1:1.57:2.41:3.59 [2]. The experiment still confirms further that concrete has different temperature rise under different pouring temperatures.

In one experiment [2], concrete mixture is prepared with a water–cement ratio of 0.45. Coarse aggregate is limestone grain of effective diameter 18 mm, while fine aggregate is natural river sand. Furthermore, selection of proper proportion of sand in sand–cement grout is necessary to make sure that the grout and the concrete mixture have the same chemical reaction velocity. Test results show that optimal sand ratio to sand–cement grout is equal to coarse aggregate ratio to concrete. Specimen is sized $25\times25\times60$ cm. In the test of heat insulation and temperature rise, three different initial temperatures, i.e., 4.4, 23.3, 40 °C, are employed.

It is shown that the concrete temperature rise changes not only with time, but also with variation of temperature field. Fig. 1 is the variation curve of concrete temperature rise recorded by the experiment under different initial temperatures [2]. Evidently, the higher the initial temperature, the faster the hydration and temperature rise will be in early age. When cement hydration course reaches a certain level, the hydration speed begins to drop; the later the concrete age, the slower the hydration speed will be, but hydration is irreversible and always goes on; after a long time, the temperature rise will be close to the largest temperature rise of concrete; the total temperature rise of concrete are the

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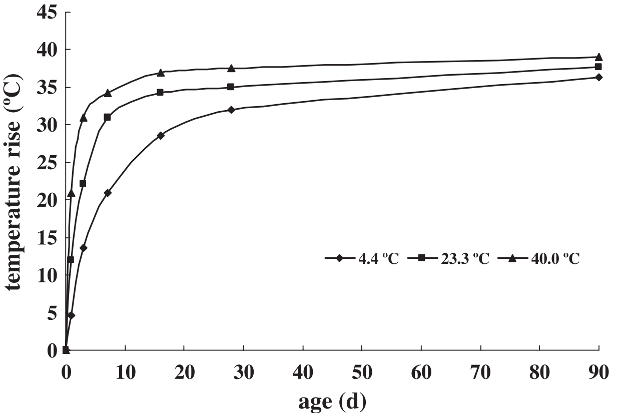

Fig. 1. Variation curve of concrete temperature rise with different initial temperatures.

same even under different initial temperatures, because the total hydration heat emitted by the same amount of cement will be the same.

2. Evaluation of current models

Most of the current models take temperature rise during hydration only as a function of concrete age [3]; among these, there are the index type (1), two-curve type (2), complex indexes type (3).

$$\theta(\tau) = \theta_0(1 - e^{-m\tau}) \tag{1}$$

$$\theta(\tau) = \frac{\theta_0\tau}{n+\tau} \tag{2}$$

$$\theta(\tau) = \theta_0\left(1 - e^{-\alpha\tau^{\beta}}\right) \tag{3}$$

where θ_0 is the eventual temperature rise, τ is concrete age, m, n, α and β are parameters depending on experimental results.

From Fig. 1, it is evident that temperature rise of concrete with identical age is different under different initial temperature. These expressions do not consider the influence of initial temperature, let alone considering the influence of temperature field change during hydration, cannot reveal the actual course of cement hydration. To show this, take one of these equations, say Eq. (1), for example. Fig. 2 is the fitted data by Eq. (3), where θ_0=26, α=0.77, β=0.47. From this figure, we get the conclusion that concrete will undergo the same temperature process no matter what its initial temperature is and that temperature rise of concrete is only related to its age; this conclusion evidently contradicts the experimental data, it is far from enough to describe the temperature process of concrete without considering initial temperature and the change of temperature during hydration.

In order to simulate the actual working state of concrete structure, it needs to have an important theoretical and engineering meaning to study the concrete temperature rise under different pouring temperatures. Based on chemical reaction dynamics, this paper considered at the same time the influence of temperature and concentration on hydration speed, and deduced the dynamic model of temperature rise caused by cementitious materials hydration.

3. Chemical reaction dynamic equation

Temperature and concentration are the major factors that affect reaction speed for the chemical reaction of common material [4–8]. The expression that describes the relation between temperature, concentration and reaction speed is called reaction dynamic equation. In general, the reaction dynamic equation can be shown with the following [4]:

$$r = f(c, T) \tag{4}$$

where r is reaction speed, c is the concentration of material participating in reaction and T is reaction temperature. There are mainly two mathematical forms of reaction dynamic equation in chemistry, i.e., the power function and two-curve type; here, we adopt the power function as the dynamic equation.

Under constant temperature in the dynamic equation of the power function, temperature and concentration had been considered to affect reaction speed independently; therefore, the equation above can be rewritten as:

$$r = f_c(c)f_T(T) \tag{5}$$

where $f_c(c)$ expresses the influence of concentration on reaction speed; $f_T(T)$ is constant k of reaction speed, expressing influence of temperature on reaction speed.

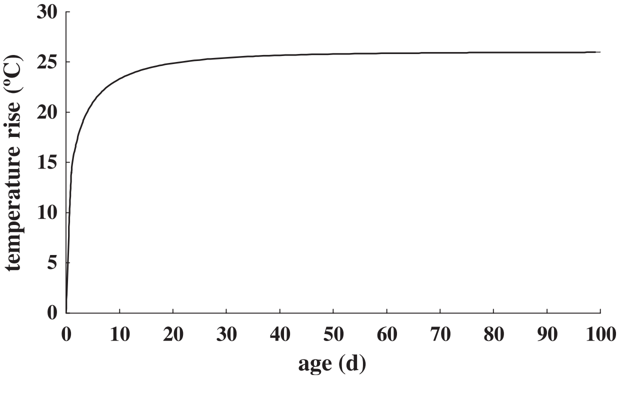

Fig. 2. Variation curve of concrete temperature rise by conventional method.

Table 1
Recorded concrete temperature rise at different initial temperatures (°C)

Initial temp (°C)	Age (days)					
	1	3	7	16	28	90
4.4	4.6	13.6	21.0	28.5	32.0	36.4
23.3	12.0	22.2	30.9	34.2	35.0	37.7
40.0	20.9	30.9	34.3	36.9	37.5	39.0

3.1. Temperature influence on reaction speed

For the most chemical reactions, the relation between reaction speed and reaction temperature can be expressed by negative index as follows [4]:

$$f_T(T) = \alpha e^{-\frac{E}{R(T+273)}} \tag{6}$$

where α is reaction factor, E is reaction activation energy, T is temperature and R=8.1344 kJ/(kmol·K) is mole gas constant. E/R is a measurement of reaction speed sensitivity to temperature, usually between 2459 and 24590 K, which needs to be determined through experiment for specific chemical reaction. Eq. (6) is the famous *Arrhenius* equation, which is deduced by Swedish chemist *Arrhenius* according to thermodynamic principles and confirmed by numerous test data.

3.2. Concentration influence on reaction speed

The influence of concentration on reaction speed can be shown with index form of concentration as follows [4]:

$$f_c(c) = c^{\beta} \tag{7}$$

where c is the concentration of material to be reacted and β is reaction order; the reaction order measures the sensitivity of reaction speed to concentration variation, the higher the reaction order, the greater the influence of concentration on reaction speed will be. Here, we assume initial concentration as 1, and the reaction completion rate or conversion rate as a, concentration c=1−a, the concentration influence on reaction speed is:

$$f_c(c) = (1-a)^{\beta} \tag{8}$$

4. Dynamic model of temperature rise caused by cementitious materials hydration

Table 2
Fitted parameters of dynamic model

θ_0	α	β_1	β_2	β_3	γ
40	2,500,000	2.8	0.001	0.0000001	4750

Table 3
Fitted concrete temperature rise at different initial temperatures (°C)

Initial temp (°C)	Age (days)					
	1	3	7	16	28	90
Dynamic model 4.4 °C	3.66	10.39	20.00	28.84	32.61	36.65
Dynamic model 23.3 °C	10.91	23.43	30.58	34.44	36.06	38.01
Dynamic model 40.0 °C	25.66	31.78	34.65	36.54	37.43	38.63
Current model	19.94	25.00	28.95	32.51	34.61	37.83

The cement hydration course is a course of chemical reaction, therefore, accords with the general law of the abovementioned chemical reaction, and the hydration speed at certain time can be shown by Eqs. Eqs. (5), (6) and (8), we get:

$$r = \alpha c^{\beta} e^{-\frac{\gamma}{T+273}}. \tag{9}$$

For given concrete, its eventual temperature rise θ_0 is not concerned with hydration course but concerned only with total heat produced during reaction course; therefore, its value is certain. It is assumed that the initial concentration of cement attending the hydration reaction is 1, the initial temperature of reaction is T_0, the temperature rise at age τ is $\theta(\tau)$, since temperature rise is directly related to heat produced during hydration, while heat produced is proportional to the quantity of cement that has undergone hydration reaction; thus, cement already reacted is proportional to temperature rise, the ratio of cement already reacted to total cement before reaction equals to that of temperature rise $\theta(\tau)$ to eventual temperature rise θ_0. Cement concentration can be expressed with the temperature rise as c=1−$\theta(\tau)/\theta_0$, hydration speed can be expressed by r=−dc/dτ=−d$\theta(\tau)/(\theta_0$d$\tau)$. According to Eq. (9), the change rate of temperature rise of hydration at τ age d$\theta(\tau)$/dτ can be expressed with the concentration and temperature at τ time as follows:

$$\frac{\mathrm{d}\theta(\tau)}{\mathrm{d}\tau} = \alpha\theta_0\left(1-\frac{\theta(\tau)}{\theta_0}\right)^{\beta} e^{-\frac{\gamma}{T+273}} \tag{10}$$

where T is actual reaction temperature at τ time, T=T_0+$\theta(\tau)$ when the reaction takes place under heat insulation; when

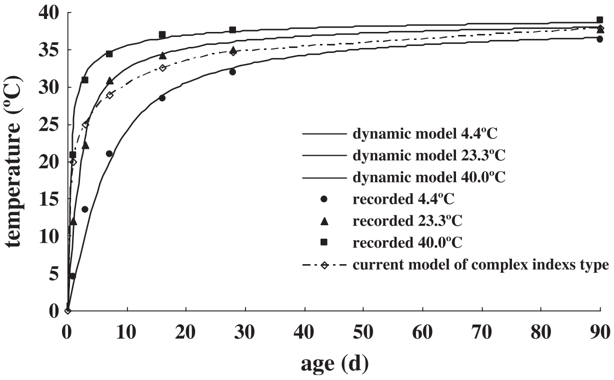

Fig. 3. Contrast of temperature rise from recorded value, dynamic model and current model.

the reaction temperature is constant, reaction order β above is also constant, but β will change when reaction temperature T changes; we assume β as quadratic polynomial of temperature, regarding it as the function of temperature, and rewrite Eq. (10) as:

$$\frac{d\theta}{d\tau} = \alpha\theta_0\left(1-\frac{\theta}{\theta_0}\right)^{\beta_1+\beta_2T+\beta_3T^2} e^{-\frac{\gamma}{T+273}} \tag{11}$$

This equation is the dynamic model of temperature rise caused by hydration. It is quite difficult to calculate temperature rise from this equation directly, so we can write it in differential form for convenience of calculation:

$$\begin{aligned}
&\theta^{(0)} = 0\\
&\theta^{(n)} = \theta^{(n-1)} + \Delta\theta^{(n)}\\
&\Delta\theta^{(n)} = \alpha\theta_0\left(1-\frac{\theta^{(n-1)}}{\theta_0}\right)^{\beta_1+\beta_2T+\beta_3T^2} e^{-\frac{\gamma}{T+273}}\Delta\tau
\end{aligned} \tag{12}$$

5. Verification

Table 1 is the experimental temperature rise of concrete at different initial temperatures corresponding to Fig. 1. Tables 2 and 3 are fitted parameter and fitted data by this model, respectively. Fig. 3 is the contrast of simulation by dynamic model with fitted parameters and recorded value of temperature rise. It is shown that this model computes accurately the temperature rise of concrete.

Normally, the concrete has heat exchange with its surroundings; therefore, the hydration of concrete is not strictly under heat insulation. If the parameter is correctly fitted, we can directly get the speed of hydration reaction at any concentration and temperature by this model; therefore, once knowing the concentration and reaction temperature of certain age, the reaction speed of this age can be directly and exactly achieved, so the model can also be used for calculation of any course of concrete temperature rise of actual dam body that has heat exchange.

From Fig. 3, with current model, only one curve can be obtained, that is to say, the processes of temperature rise are the same with different initial temperatures, because the current model takes the temperature rise as a function of concrete age only, which neglects the impact of initial temperature. However, the Dynamic Model can reflect the real course of temperature rise according to initial temperature and temperature rise during hydration.

6. Conclusion

(1) Concrete undergoes different temperature rise processes under different pouring temperatures or different initial temperatures. The concrete temperature rise changes not only with time, but also with variation of temperature field.

(2) At present, there are many models for computation of temperature rise caused by cementitious materials hydration, but the most takes this temperature rise as a function of concrete age only, without considering the impact of initial temperature and temperature rise during hydration, and thus cannot reflect the real course of temperature rise.

(3) Deduced from the basic nature of chemical change, the dynamic model of temperature rise caused by cementitious materials hydration not only accords with the general law of chemical change, but also coincides well the experimental data and stimulates well the actual course of temperature rise of concrete under any initial temperature; in addition, it can be used to calculate the actual temperature process of concrete with heat exchange.

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