# Numerical simulation of heat transfer and moisture transport in high performance concrete at early age

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ABSTRACT: A hygro-thermo-chemical model (Di Luzio & Cusatis 2009a) for high-performance concrete (HPC) suitable for the analysis of moisture transport and heat transfer at the early age and beyond is presented. The model formulation exploits the two classical macroscopic mass and energy conservation laws, which are written by using humidity and temperature as primary variables and by taking into account explicitly various chemical reactions, such as cement hydration, silica fume reaction, and silicate polymerization. The present model can simulate early age phenomena, such as self-heating and self-desiccation, with great accuracy as the comparison with experimental test data has demonstrated (Di Luzio & Cusatis 2009b).

# 1 INTRODUCTION

Nowadays, the durability of concrete constructions is one of the most important issues in the civil engineering field. The introduction of highperformance concrete (HPC) mixes does not settle the problem of cracking (especially at the very early age). Reliable and predictive analyses of the behavior of concrete structures at early ages (and beyond) require the formulation of a consistent theoretical framework that includes all of the various phenomena characterizing early age evolution of concrete. Many experimental, theoretical, and computational studies on the behavior of concrete at the early age and, specifically, on self-heating and self-desiccation can be found in the literature; among others, Wittmann (2002), Ulm & Coussy (1995), Cervera et al. (1999), Bažant et al. (2003), Gawin et al. (2006), and Oh & Cha (2003). Typical HPC mixes are characterized by low water-tocement ratio, high cement content, and by the incorporation of silica fume (SF) or other pozzolanic materials (Mazloom et al. 2004). Both pozzolanic reaction and silicate polymerization interact with cement hydration (Taylor 1997) influencing concrete mesostructure and, ultimately, concrete behavior. None of the analytical models currently available in the literature can simulate the effect of SF reaction and polymerization on heat transfer and moisture transport in concrete.

The objective of this paper is to present a brief summary of the advances in the hygro-thermochemical modelling of HPC recently achieved by the authors (see for details Di Luzio & Cusatis, 2009a,b).

# 2 GOVERNING EQUATIONS

# 2.1 Moisture transport

Water can be found in concrete in various phases: (a) capillary water, (b) water vapor, (c) adsorbed water, and (d) non-evaporable (chemically bound) water (Powers & Brownyard 1946). The transport mechanisms of each phase are completely different and they are influenced by concrete microstructure, which means they depend on the extent of the chemical reactions. In principle, the different water mechanisms should transport be modeled independently but the complexity of the phenomena hampers this kind of approach and calls for a simplified approximated analysis. First of all, it is possible to simplify the problem by postulating the existence of local thermodynamic equilibrium (Bažant 1970, Gawin et al. 2006, among others), since the characteristic times of the water transport mechanisms are much smaller than those associated with concrete chemical reactions. In this study, as widely accepted in the literature, the overall moisture process under transport isothermal conditions is described through the Fick's law that expresses the flux of water mass per unit time J as proportional to the spatial gradient of the relative humidity h

$$\boldsymbol{J} = -\boldsymbol{D}(\boldsymbol{h}, \boldsymbol{T})\nabla\boldsymbol{h} \tag{1}$$

The proportionality coefficient D(h,T) is called moisture permeability and it is a nonlinear function of the relative humidity h and temperature T (Bažant & Najjar 1972). The moisture mass balance requires that the variation in time of the water mass per unit volume of concrete (water content w) be equal to the divergence of the moisture flux J

$$-\frac{\partial w}{\partial t} = \nabla \bullet \boldsymbol{J} \tag{2}$$

The water content w can be expressed as the sum of the evaporable water  $w_e$  (capillary water, water vapor, and adsorbed water) and the non-evaporable (chemically bound) water  $w_n$  (Mills 1966. Pantazopoulo & Mills 1995). It is reasonable to assume that the evaporable water is a function of relative humidity, h, degree of hydration,  $\alpha_c$ , and degree of silica fume reaction,  $\alpha_s$ , i.e.  $w_e = w_e(h, \alpha_c, \alpha_s)$ age-dependent sorption/desorption isotherm (Norling Mjonell 1997). Under this assumption and by substituting Equation 1 into Equation 2 one obtains

$$-\frac{\partial w_e}{\partial h}\frac{\partial h}{\partial t} + \nabla \bullet (D_h \nabla h) = \frac{\partial w_e}{\partial \alpha_c} \partial \xi_c + \frac{\partial w_e}{\partial \alpha_s} \partial \xi_s + \mathcal{H}_n \qquad (3)$$

where  $\partial w_e / \partial h$  is the slope of the sorption/desorption isotherm (also called moisture capacity). The governing equation (Equation 3) must be completed by appropriate boundary and initial conditions.

The relation between the amount of evaporable water and relative humidity is called "adsorption isotherm" if measured with increasing relativity humidity and "desorption isotherm" in the opposite case. Neglecting their difference (Xi et al. 1994), in the following, "sorption isotherm" will be used with reference to both sorption and desorption conditions. By the way, if the hysteresis of the moisture isotherm would be taken into account, two different relation, evaporable water vs relative humidity, must be used according to the sign of the variation of the relativity humidity. The shape of the sorption isotherm for HPC is influenced by many parameters, especially those that influence extent and rate of the chemical reactions and, in turn, determine pore structure and pore size distribution (water-to-cement ratio, cement chemical composition, SF content, curing time and method, temperature, mix additives, etc.). In the literature various formulations can be found to describe the sorption isotherm of normal concrete (Xi et al. 1994). However, in the present paper the semi-empirical expression proposed by Norling Mjornell (1997) is adopted because it explicitly accounts for the evolution of hydration reaction and SF content. This sorption isotherm reads

$$w_{e}(h,\alpha_{c},\alpha_{s}) = G_{1}(\alpha_{c},\alpha_{s}) \left[1 - \frac{1}{\frac{10(g_{1}\alpha_{c}^{\infty} - \alpha_{c})h}{e^{10(g_{1}\alpha_{c}^{\infty} - \alpha_{c})h}}}\right] + (4)$$
$$K_{1}(\alpha_{c},\alpha_{s}) \left[e^{10(g_{1}\alpha_{c}^{\infty} - \alpha_{c})h} - 1\right]$$

where the first term (gel isotherm) represents the physically bound (adsorbed) water and the second term (capillary isotherm) represents the capillary water. This expression is valid only for low content of SF. The coefficient  $G_1$  represents the amount of water per unit volume held in the gel pores at 100% relative humidity, and it can be expressed (Norling Mjornell 1997) as

$$G_{1}(\alpha_{c},\alpha_{s}) = k_{vg}^{c}\alpha_{c}c + k_{vg}^{s}\alpha_{s}s$$
(5)

where  $k_{vg}^{c}$  and  $k_{vg}^{s}$  are material parameters. From the maximum amount of water per unit volume that can fill all pores (both capillary pores and gel pores), one can calculate  $K_{l}$  as one obtains

$${}_{K_{1}}\left(\alpha_{c},\alpha_{s}\right) = \frac{{}^{W_{0}-0.188\alpha_{c}s+0.22\alpha_{s}s-G_{1}}\left[1-e^{10\left(g_{1}\alpha_{c}^{\infty}-\alpha_{c}\right)h\right]}}{{}^{10\left(g_{1}\alpha_{c}^{\infty}-\alpha_{c}\right)h}_{-1}}$$
(6)

The material parameters  $k_{vg}^c$  and  $k_{vg}^s$  and  $g_1$  can be calibrated by fitting experimental data relevant to free (evaporable) water content in concrete at various ages (Di Luzio & Cusatis 2009b).

#### 2.2 Temperature evolution

Note that, at early age, since the chemical reactions associated with cement hydration and SF reaction are exothermic, the temperature field is not uniform for non-adiabatic systems even if the environmental temperature is constant. Heat conduction can be described in concrete, at least for temperature not exceeding 100°C (Bažant & Kaplan 1996), by Fourier's law, which reads

$$q = -\lambda \nabla T \tag{7}$$

where q is the heat flux, T is the absolute temperature, and  $\lambda$  is the heat conductivity; in this

study, an average value of  $\lambda$ =2.3 W/m °C (Bažant & Kaplan 1996) is used in the numerical simulations. The enthalpy balance equation can be written as

$$\rho c_t \frac{\partial T}{\partial t} = -\nabla \bullet \boldsymbol{q} + \mathcal{Q}_c^{\boldsymbol{x}} + \mathcal{Q}_s^{\boldsymbol{x}} + \mathcal{Q}_p^{\boldsymbol{x}}$$
(8)

where q is the mass density of concrete, and  $c_t$  is the isobaric heat capacity (specific heat) of concrete (an average value of  $c_t$ =1100 J/kg °C can be generally adopted for all concretes, Neville 1997). Q c, Q s, and  $Q_{p}$  represent the rate of heat generation per unit volume due to cement hydration, SF reaction, and silicate polymerization, respectively. Since, to the best of the authors knowledge, there is no evidence of temperature variation associated with the polymerization of silicates,  $Q_{p}=0$  is adopted hereinafter. If one assumes, as commonly accepted in the literature (Ulm & Coussy 1995, Cervera et al. 1999, Gawin et al. 2006) and confirmed by various theoretical and experimental investigations (Bentz & Stutzman 1994), that the latent heat of hydration reaction per unit of hydrated mass  $(Q^{\sim}_{c})$  is constant for a given concrete, then one can write (Cervera et al. 1999)

$$\mathcal{Q}_{c}^{\mathbf{x}} = c \, \mathcal{Q}_{c}^{\mathbf{x}} \, \widetilde{\mathcal{Q}}_{c} \qquad \text{and} \qquad \mathcal{Q}_{s}^{\mathbf{x}} = s \, \mathcal{Q}_{s}^{\mathbf{x}} \, \widetilde{\mathcal{Q}}_{s} \tag{9}$$

where  $\alpha_c$  is the rate of the hydration degree discussed, c is the cement mass content,  $\alpha_s$  is the rate of pozzolanic reaction degree, s is the SF mass content, and  $Q_s$  is the latent heat of SF reaction per unit mass of reacted SF. The hydration enthalpy,  $Q_c$ , typically ranges from 400 kJ/kg to 550 kJ/kg, depending upon cement composition (Bentz et al. 1998). The enthalpy of SF reaction,  $Q_s$ , can be assumed to be constant and equal to 780 kJ/kg (Waller et al. 1996).

By substituting Equations 7 and 9, into Equation 8 one obtains

$$\nabla \bullet (\lambda \nabla T) - \rho c_t \frac{\partial T}{\partial t} + c \mathscr{A}_c \widetilde{Q}_c + s \mathscr{A}_s \widetilde{Q}_s = 0$$
(10)

This energy conservation equation must be completed by appropriate boundary and initial conditions.

### 3 CHEMICAL MODEL

#### 3.1 Cement hydration

Cement hydration is characterized by the reaction of free-water with unhydrated cement particles, which mainly produces calcium silicates hydrates (CSH), calcium hydroxide (CH), ettringite (Aft), and monosulfate (Afm) (Taylor 1997). Because the exact stoichiometry of the chemical reactions involved is not known (Taylor 1997, Neville 1997), in the literature many authors (Ulm & Coussy 1995, de Schutter & Taerwe 1995, van Breugel 1992) have studied cement hydration with reference to an overall hydration process. The present study adopts this approach and, in particular, the thermodynamics based model proposed by Ulm and Coussy (1995) and later revisited by Cervera et al. (1999) and by Gawin et al. (2006), according to which the evolution equation of the hydration degree has the following expression

$$a_{c}^{k} = A_{c}\left(\alpha_{c}\right)\beta_{h}(h) e^{-E_{ac}/RT}$$
(11)

where

$$A_{c}\left(\alpha_{c}\right) = A_{c1}\left(\frac{A_{c2}}{\alpha_{c}^{\infty}} + \alpha_{c}\right)\left(\alpha_{c}^{\infty} + \alpha_{c}\right)e^{-\eta_{c}\alpha_{c}/\alpha_{c}^{\infty}}$$
(12)

$$\beta_{h}(h) = \left[1 + (a - ah)^{b}\right]^{-1}$$
(13)

where  $A_c$  is the so-called normalized chemical affinity, the function  $\beta_h$  is an empirical function,  $E_{ac}$ is the hydration activation energy, R is the universal gas constant, and  $\eta_c$ ,  $A_{cl}$ , and  $A_{c2}$  are material parameters. The ratio  $E_{ac}/R$  can be experimentally determined and it ranges from 3000 to 8000 K for concrete. In the present study the value Eac/R=5000K will be adopted when specific measurements are not available. The parameters  $\eta_c$ ,  $A_{cl}$ , and  $A_{c2}$  can be calibrated, for example, by simulating the temperature evolution during adiabatic tests. The parameters a and b can be calibrated through the analysis of experimental data but the constant values a=5:5 and b=4 can be generally adopted (Gawin et al. 2006, Bažant & Prasannan 1989)

#### 3.2 Silica fume reaction

A certain amount of SF is often added in concrete mixture in order to produce HPC (Persson 1998). SF belongs to the category of highly pozzolanic materials and it consists of silica in no crystalline form with a high specific surface and exhibiting high pozzolanic activity. The effect of SF on moisture transport phenomena is here modeled through the introduction of the degree of SF reaction,  $\alpha_s$ , defined as the ratio between the amount of reacted SF and the total amount of SF. Since the kinetics of the pozzolanic reaction can be assumed to be a diffusion controlled process (Wild et al. 1995, Zelić et al. 2000), the theory adopted in the previous Section to describe cement hydration can be exploited to describe the evolution of SF reaction (Yajun & Cahyadi 2004). Accordingly, one has

$$a_{s}^{k} = A_{s}\left(\alpha_{s}\right)e^{-E_{as}/RT}$$
(14)

where

$$A_{s}\left(\alpha_{s}\right) = A_{s1}\left(\frac{A_{s2}}{\alpha_{s}^{\infty}} + \alpha_{s}\right)\left(\alpha_{s}^{\infty} + \alpha_{s}\right)e^{-\eta_{s}\alpha_{s}^{-}/\alpha_{s}^{\infty}}$$
(15)

where  $A_s$  is the SF normalized affinity,  $E_{as}$  is the activation energy of SF reaction and  $\alpha_s$  is the asymptotic value of SF reaction degree.  $E_{as}/R=9700$  K can be generally assumed (Bentz et al. 1998). The material parameters  $A_{s1}$ ,  $A_{s2}$ , and  $\eta_s$  can be calibrated similarly to the parameters governing cement hydration (Di Luzio & Cusatis 2009b). When a sufficient amount of SF is available in concrete, all the CH produced by cement hydration can be consumed by the pozzolanic reaction. Considering the data of Persson (2002), the asymptotic value of SF reaction degree can be estimated as (see for details Di Luzio & Cusatis 2009a)

$$\alpha_s^{\infty} = SF^{eff} \min\left[1, \frac{\min\left(0.16; 0.4w/c\right)}{s/c}\right]$$
(16)

where  $SF^{eff}$  is the "efficiency" of SF, i.e. the mass ratio between the SiO<sub>2</sub> mass content and the total mass of SF (typically  $SF^{eff}$  ranges from 0.85 to 0.92, Taylor 1997).

#### 3.3 Silicate polymerization

Many experimental investigations (Taylor 1997) revealed that CSH particles bond together over time, increasing the average degree of polymerization of the silicate chains and causing the CSH to become stiffer, stronger, and denser. The key reaction for linking the CSH gel hydrolyzed molecules together is the condensation, in which two monomers are connected to form a polymeric cluster and water is "condensed" out. Silicate polymerization is much more pronounced in the presence of SF because the SF pozzolanic reaction increases the content of CSH gel. When the water consumed by cement hydration is less than the water condensed by silicate polymerization, one can observe a reduction of the non-evaporable water content starting after 2–3 months (Zhang & Gjorv 1991)

The polymerization process can be modeled through the relative concentration of silicate polymers,  $\alpha_p$ , defined as the ratio between the mass of polymeric species and the mass of CSH gel. The rate of the relative concentration of silicate polymers can be formulated as

$$a_{p}^{k} = A_{p1} A_{p}\left(\alpha_{p}\right) B_{p}\left(\alpha_{c}\right) e^{-E_{ap}/RT}$$
(17)

where

$$A_p(\alpha_p) = \alpha_p^{\infty} - \alpha_p$$
 and  $B_p(\alpha_c) = H(\alpha_c - \alpha_c^0)$  (18)

the coefficient  $A_p$  expresses the fact that the rate of polymerization is reduced as polymerization progresses and it eventually vanishes when the polymerization is complete, the coefficient  $B_p$  takes into account the effect of cement hydration (hydration products need to be present for the polymerization to occur), and H is the Heaviside step function, used here to set a threshold value of  $\alpha^{\theta}_{c}$ , below hydration degree, which the polymerization process can be neglected (the value of 0:1 is adopted). In this study it is assumed an averaged value of 50 kJ/mol for the Arrhenius energy, which gives  $E_{ap}/R=6000$  K. The material parameter  $A_{p1}$  can be calibrated on the basis of experimental data on the evolution of the polymerized species.

#### 3.4 Asymptotic hydration degree

The asymptotic (ultimate) hydration degree,  $\alpha_c^{\infty}$ , is always less than one (Bentz et al. 1998). Pantazopoulo and Mills (1995) proposed to calculate  $\alpha_c^{\infty}$  on the basis of a mass balance between water needed to ensure saturation conditions and total water content, and they obtained

$$\alpha_{c}^{\infty} = \frac{1.031 \, w/c}{0.194 + w/c} \tag{19}$$

The presence of SF further reduces the ultimate achievable hydration degree because, due to the formation of additional CSH gel from the pozzolanic reaction, extra water is hindered into the gel pores and it becomes unavailable for cement hydration (Bentz et al. 1998). In addition, the specific surface of the CSH gel increases and unhydrated cement grain cores become less accessible. Considering the effect of SF on the water balance equation at saturation, one can rewrite Equation (19) as

$$\alpha_{c}^{\infty} = \frac{1.031 \, w \, / \, c - 0.279 \, \left( s \, / \, c \right) \alpha_{s}^{\infty}}{0.194 + w \, / \, c} \tag{20}$$

where s is SF content and  $\alpha^{\infty}_{s}$  is the asymptotic SF reaction degree given by Equations 11 and 12. The asymptotic degree of hydration must be positive and so Equation 16 holds only if  $w/c>0.27(s/c) \alpha^{\infty}_{s}$ .

#### 3.5 Nonevaporable water

As discussed previously, the non-evaporable water is the amount of water that is chemically bound as consequence of cement hydration, SF reaction, and silicate polymerization. In general, one can write

$$w_n\left(\alpha_c,\alpha_s,\alpha_p\right) = \kappa_c c \alpha_c + \kappa_s s \alpha_s - \alpha_c\left(\kappa_{pc} c + \kappa_{ps} s\right)$$
(21)

The coefficient  $\kappa_c$  is the mass ratio of nonevaporable water at full hydration,  $\kappa_c$ =0:253, (Powers 1964, Mills 1966, Norling Mjonell 1997). The second term represents the effect of SF reaction and, as assumed in this formulation, it is equal to 0. The third term characterizes the effect of polymerization and the negative sign traduces the fact that during silicate polymerization water is released in the system and the chemically bound water is reduced. For regular concrete mixes without the addition of SF the effect of the polymerization is rather small and it can be neglected by assuming  $\kappa_{pc}$ =0. On the contrary the value of  $\kappa_{ps}$  cannot be assumed equal to zero and must be determined from the analysis of experimental data.

#### **4 PERMABILITY**

Moisture diffusion in concrete depends on various diffusion mechanisms that characterize the mobility of different water phases present in concrete and that are influenced by the pore structure of concrete. In this work, as typically done in the literature (Bažant & Najjar 1972), the diffusion mechanisms are described phenomenologically through Fick's law (Equation 1) which is characterized by the moisture permeability. The proposed formula for the moisture permeability is given by

$$D(h,T) = \psi(T)D_1 \left[ 1 + \left(\frac{D_1}{D_0} - 1\right) (1-h)^n \right]^{-1}$$
(22)

where

$$D_{0} = \widetilde{D}_{0} \left(\frac{w}{c}\right)^{3} \left(1 - \frac{s}{c}\right)^{2}; \quad D_{1} = \widetilde{D}_{1} \left(\frac{w}{c}\right)^{2.5} \left(1 - \frac{s}{c}\right)^{2} (23)$$

$$\psi(T) = \exp\left(\frac{E_{ad}}{RT_0} - \frac{E_{ad}}{RT}\right)$$
(24)

The coefficient  $\psi(T)$  takes into account the effect of temperature on permeability as earlier proposed by Bažant and Najjar (1972),  $D_0$  and  $D_1$  represent moisture permeability for a completely dry situation and completely saturated situation, respectively. The exponent *n* governs the rate at which permeability gradually changes from  $D_0$  to  $D_1$ . The exponents of the power laws in Equation 19 have been obtained by analyzing drying data gathered from the literature (Di Luzio & Cusatis 2009b). In Equation 20, *T* is the absolute temperature,  $T_0$  is the reference room temperature (Bažant & Najjar 1972).

#### 5 NUMERICAL SIMULATIONS

The numerical implementation, the parameter calibration and an extensive validation of the proposed model is presented in Di Luzio & Cusatis (2009b). In the following two numerical simulations concerning the self-heating, self-desiccation and drying are considered. A more extensive verification can be found in Di Luzio & Cusatis (2009b) in which temperature rise and self- desiccation are also evaluated simultaneously.

The first example concerns the experimental investigation of Bentz et al. (1998) on conventional and high-performance concretes aimed at the characterization of their adiabatic heat. The values  $Q \sim = 520 \text{ kJ/kg}, E_{ac}/R = 5490 \text{ K}; \text{ and } E_{as}/R = 9620 \text{ K}$ can be assumed for all mixes based on data reported in Bentz et al. (1998). The optimized parameters are reported in the first column of Table 1. Figure 1 show the comparison between the experimental data and the numerical simulations. Symbols are the experimental data points, lines represent the results obtained by the present model with (solid line) and without (dashed line) the effect of the SF reaction degree. These results clearly show that the proposed model can be reliably employed to predict the temperature rise and the heat production of a wide variety of concrete mixes with and without SF.

The second example concerns the experimental investigations of Kim and Lee (1999) on self-desiccation and moisture drying at early ages. They measured the non-uniform moisture distributions in concrete samples of three different concrete mixes exposed to ambient air with 50% relative humidity. The three mixes were characterized by cement content, water-to-cement ratio, and density equal to 541, 423, 310 kg/m<sup>3</sup>, 0.28, 0.4, 0.68, and 2394, 2344, 2257 kg/m<sup>3</sup>, respectively. The tested specimens

Table 1. Values of the parameters used in the numerical simulations.

Par.(unit)	Example 1	Example 2	
$\overline{g_1(-)}$	1.5	1.2	
$\tilde{k}^{c}_{vg}(-)$	0.2	0.255	
$k^{s}_{vo}(-)$	0.36		
$A_{cl}(h^{-1})$	$20.10^{7}$	$1.5 \cdot 10^{7}$	
$A_{c2}(-)$	$1 \cdot 10^{-6}$	$5 \cdot 10^{-2}$	
$\eta_c(-)$	6.5	8	
$A_{sl}(\mathbf{h}^{1})$	$5 \cdot 10^{7}$		
$A_{s2}(-)$	$1 \cdot 10^{-6}$		
ηs (-)	9.5		
$\dot{C}_p(\mathbf{h}^{-1})$			
$D_0(m^2/h)$		0.085	
$D_1(m^2/h)$		6	
n(-)		3	



Figure 1. Experimental investigation of Bentz et al. (1998): experimental (data points) and numerical (solid lines) adiabatic temperature rise curves for concrete with different values of water-to-cement ratio and SF content.



Figure 2. Numerical simulations of the experimental data of Kim and Lee (1999): relative humidity vs. time due to self-desiccation, (a) and (b), and due to moisture diffusion and self-desiccation, (c) to (h).

were prisms of dimensions 10x10x20 cm, which were moist-cured before drying. Two different ages were considered:  $t_0=3$  and 28 days. The internal relative humidity was measured at the distance of 3, 7, and 12 cm from the exposed surface, which was one of the 10x10 cm square bases. The other five sides were sealed to generate a uniaxial moisture diffusion. In addition, completely sealed cubic specimens were also used to measure the variation of relative humidity due to self-desiccation only. The numerical simulations of these tests were performed by using the plane finite element mesh and the results are shown in Figure 2. The optimized parameters are reported in the second column of Table 1. The agreement is overall excellent, proving that the present model can be used reliably to estimate moisture diffusion in normal and highperformance concretes.

## 6 CONCLUSION

In this study a hygral-thermo-chemical model for the simulation of moisture transport and heat transfer in HPC has been presented. The model is characterized by only one moisture transport equation governing the evolution of pore relative humidity which is coupled with the heat balance equation which describes the evolution of temperature and takes into account the heat released during hydration and silica fume reaction. The aging effect associated with the silica fume is modeled through the degree of pozzolanic reaction. The aging effect of silicate polymerization is modeled introducing the concentration of silicate polymers (Di Luzio & Cusatis 2009a). The chemically bound (non evaporable) water is modeled through an expression that takes into account hydration and silicate polymerization. Extensive calibration and validation of the present formulation (Di Luzio & Cusatis 2009b), examples of which are reported in this paper, showed the superior capability of the presented model to simulate and predict the hygro-thermochemical behavior of HPC at early age.

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