

# Behavior of Ultra High Performance Concrete at Early Age: Experiments and Simulations

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## Abstract

Ultra-high performance concrete (UHPCs) are cementitious composite materials with high level of performances reached by a low water-binder ratio, an optimized gradation curve, and with the use of thermal activation. In the past decades, various UHPC's have been developed and utilized, however, very limited research is conducted studying their early age strength development. Hence, a comprehensive mathematical model capable of describing the early age effects is needed to facilitate construction planning and reliability assessments. The literature will show the experimental characterization as well as the results of subsequent aging simulations utilizing and coupling the Hygro-Thermo-Chemical model and the Lattice Discrete Particle Model with aging effects (HTC-A-LDPM) for a UHPC at various early ages. Investigated tests include unconfined compression, cylinder Brazilian, and beam three-point-bending. The HTC component of the computational framework allows taking into account various curing conditions as well as known material constituents and predicts the concrete maturity. The LDPM component, which is a discrete mechanical model, simulates the failure behavior of concrete at the coarse aggregate mesoscale level. Connecting the two components, the aging functions are developed with great simplicity to compute accurately the material properties. The proposed hygro-thermo-chemo-mechanical coupled early age framework (HTC-A-LDPM) can comprehensively capture cement hydration effects as well as strength development for the UHPC. Furthermore, with the comprehensively calibrated and validated aging model, size effect simulations and predictions of various early ages and sizes are carried out in furtherance of an experimental campaign.

## Keywords

UHPC, Concrete, Early Age, Material Characterization, Strength Gain, Discrete Model

## 1 Introduction

Ultra high performance concretes (UHPCs) are cementitious composites characterized by high compressive strength, typically greater than 150 MPa (21.7 ksi), by low water-to-binder ratio, optimized particle size distribution, thermal activation, and fiber reinforcement. Moreover, UHPC has a discontinuous pore structure that reduces liquid ingress and permeability, significantly enhancing durability as compared to normal and high-performance concretes.

With the increased adoption of UHPC materials in the construction industry, also the demand for computational models that can be utilized in design is rising. Di Luzio and Cusatis [2009] formulated, calibrated, and validated the Hygro-Thermo-Chemical (HTC) model suitable for the analysis of moisture transport and heat transfer for cement based concrete. Classical macroscopic mass and energy conservation laws are written in terms of humidity and temperature as primary variables and by taking into account explicitly various chemical reactions, such as cement hydration and silica fume reaction [DiLuzio & Cusatis 2009]. Furthermore, Di Luzio and Cusatis [2013], coupled the HTC model with the microplane model and the solidification-microprestress theory [Bazant 1989] taking into account creep, shrinkage, thermal deformation, and cracking of concrete at early age.

While finite element solvers are broadly used for analyzing the mechanical behavior of concrete structures, the Lattice Discrete Particle Model (LDPM) [Cusatis 2011] is better in simulation of the failure behavior of concrete. LDPM simulates concrete at the length scale of coarse aggregate pieces (mesoscale) and is formulated within the framework of discrete models, which enable capturing the salient aspects of material heterogeneity while keeping the computational cost manageable [Cusatis 2011].

The HTC and LDPM models are selected as basis for the presented early age model for concrete. The HTC model can comprehensively capture the hygral and thermal evolutions and chemical reactions during aging. The LDPM model, on the other hand, can provide great insights into the concrete behavior on the mesoscale level and also simulate well the mechanical behavior of concrete structures under various loading conditions at the macroscopic level. The two models are bridged by introducing proper aging functions for the LDPM parameters.

## 2 Experimental Characterization of Early Age Behavior of UHPC

The material composition of the adopted UHPC consists of LaFarge Type H cement, F-50 sand, Sil-co-sil 75 silica flour, Elkem ES-900W silica fume, ADVA-190 Superplasticizer, and tap water. The maximum particle size, 0.6 mm, is limited to that of silica sand [Roth et al. 2009]. Two curing protocols with and without hot water bath curing were utilized. A first group of specimens were kept in a humidity room (HR) for 14 days. A second group, instead, was kept in a humidity room for 7 days after which the specimens were placed in a hot water bath (WB) at 85°C for another 7 days. Both groups were let to dry at constant laboratory conditions (about 22 °C and 50% RH). Unconfined compression tests using 2×2” (50.8×50.8 mm in height and diameter) cylinders, three-point-bend (TPB) tests with half-depth notched 1×1×5” (25.4×25.4×127 mm) beams, and tensile splitting tests using 3×1” (76.2×25.4 mm) disks were carried out on nominal ages of 3, 7, 14, and 28

days. Circumferential expansion control for compression tests and crack mouth opening displacement (CMOD) control for three-point bending and splitting tests were utilized to obtain full post-peak behavior. Furthermore, boundary effects in compression tests were reduced by applying dry-moly lubricant.

In order to calibrate the HTC model, RH measurements inside specimens as well as of ambient environment were conducted with three curing routines: 14 days HR, 7 days HR + 7 days WB, and fully sealed (self desiccation) at room temperature, each using five 2x2" (50.8x50.8 mm) cylinders, with compact coupled RH sensors. At the time of casting, a straw with one end closed and the other covered by nylon net was vertically inserted into each specimen with the perforated end centered in the specimen. After humidity room curing, the closed end of the straw was opened up and sealed again housing a RH sensor in the perforated area, which remains sealed during data recording. Self desiccation specimens were sealed with plastic molds.

### **3 Computational Framework for the Simulation of UHPC at Early Age**

The proposed hygro-thermo-chemo-mechanical coupled early age model for concrete consists of two main components: HTC model and LDPM model, linked by aging functions. The behavior of concrete at early age heavily depends on moisture transport and heat transfer, which can be calculated by imposing moisture mass balance and enthalpy balance equations in the volume of interest [DiLuzio & Cusatis 2013]. Arrhenius type of equations are found to govern cement hydration, pozzolanic reactions, and silicate polymerization [DiLuzio & Cusatis 2009], which are adopted in HTC to calculate an overall aging degree of concrete. The LDPM, on the other hand, simulates the concrete mesostructure on the scale of coarse aggregates. The lattice system which represents the mesostructure topology is defined by a Delaunay tetrahedralization of the particle centers. Mesostructure deformation is described in LDPM through the adoption of rigid-body kinematics [Cusatis 2011].

#### **3.1 Hygro-Thermo-Chemical (HTC) model**

##### **3.1.1 *Moisture Transport and Heat Transfer***

The overall moisture transport, including water in various phases [Powers 1946] is described through Fick's law that expresses the flux of water mass per unit time  $\mathbf{J}$  as a function of the spatial gradient of the relative humidity  $h$ . The moisture mass balance requires the change in water content  $dw$  to be equal to the divergence of moisture flux  $\mathbf{J}$ . The water content  $w$  is the sum of evaporable water  $w_e$  (capillary water, water vapor, and absorbed water) and non-evaporable (chemically bound) water  $w_n$  [Mills 1966, Panta 1995]. Assuming that  $w_e$  is a function of relative humidity  $h$ , degree of hydration  $\alpha_c$ , and degree of silica fume reaction  $\alpha_s$ , one can write  $w_e = w_e(h, \alpha_c, \alpha_s)$  as age-dependent sorption/desorption isotherm [Norling 1997]. By mathematical substitution, the moisture balance equation relating hydration/reaction degrees [DiLuzio & Cusatis 2009] is achieved:

$$\nabla \cdot (D_h \nabla h) - \frac{\partial w_e}{\partial h} \frac{\partial h}{\partial t} - \left( \frac{\partial w_e}{\partial \alpha_c} \dot{\alpha}_c + \frac{\partial w_e}{\partial \alpha_s} \dot{\alpha}_s + \dot{w}_n \right) = 0 \quad (1)$$

Similarly, heat conduction in concrete can be expressed, at least for a temperature not exceeding 100 ° C [Bazant 1996], based on Fourier's Law:

$$\nabla \cdot (\lambda_t \nabla T) - \rho c_t \frac{\partial T}{\partial t} + \dot{\alpha}_s s \tilde{Q}_s^\infty + \dot{\alpha}_c c \tilde{Q}_c^\infty = 0 \quad (2)$$

where  $\tilde{Q}_c^\infty$  = hydration enthalpy, and  $\tilde{Q}_s^\infty$  = latent heat of silica-fume reaction per unit mass of reacted silica-fume.

### 3.1.2 Cement Hydration and Silica Fume Reaction

With the assumption that the thermodynamic force conjugate to the hydration extent, named the *chemical affinity*, is governed by an Arrhenius-type equation and that the viscosity governing the diffusion of water through the layer of cement hydrates is an exponential function of the hydration extent [Ulm 1995], Cervera et al. [1999] proposed the evolution equation for the hydration degree:  $\dot{\alpha}_c = A_c(\alpha_c) e^{-E_{ac}/RT}$ , and  $A_c(\alpha_c) = A_{c1} \left( \frac{a_{c2}}{\alpha_c^\infty} + \alpha_c \right) (\alpha_c^\infty - \alpha_c) e^{-\eta_c \alpha_c / \alpha_c^\infty}$ , where  $\alpha_c^\infty$  is the asymptotic degree of hydration,  $A_c(\alpha_c)$  is the *normalized chemical affinity*,  $E_{ac}$  is the hydration activation energy,  $R$  is the universal gas constant, and  $\eta_c$ ,  $A_{c1}$ , and  $A_{c2}$  are material parameters [DiLuzio & Cusatis 2009]. To account for the situation that the hydration process slows down and may even stop if the relative humidity decreases below a certain value ( $h \approx 75\%$ ), the equation can be rewritten as:  $\dot{\alpha}_c = A_c(\alpha_c) \beta_h(h) e^{-E_{ac}/RT}$ , where  $\beta_h(h) = [1 + (a - ah)^b]^{-1}$ . The function  $\beta_h(h)$  is an empirical function that was first proposed for the definition of the equivalent hydration period by Bazant and Prasanna [1989]. The parameters  $a$  and  $b$  can be calibrated by comparison with experimental data but values  $a = 5.5$  and  $b = 4$  can be generally adopted [Bazant 1989, Gawin 2006]. The theory adopted for cement hydration can be as well utilized for silica fume (SF) reaction since pozzolanic reactions can also be assumed to be diffusion controlled. Accordingly, the degree of SF reaction  $\alpha_s$  is introduced [DiLuzio & Cusatis 2009].

### 3.1.3 Aging Degree

Experimental studies show that the strength evolution at early age depends not only on the degree of chemical reactions, but also on the kinetics of the reactions, e.g. relative humidity and curing temperature [Cervera 2000]. The aging degree  $\lambda$  is formulated such that it approaches the normalized asymptotic value of 1 at time of infinity [Cervera 1999], correspondingly the material properties, which can be assumed to depend on the aging degree, also go to asymptotic values when concrete fully cures:

$$\dot{\lambda} = \left( \frac{T_{max} - T}{T_{max} - T_{ref}} \right)^{n_\lambda} (B_\lambda - 2A_\lambda \alpha) \dot{\alpha} \quad (3)$$

where  $B_\lambda = [1 + A_\lambda(\alpha_\infty^2 - \alpha_0^2)] / (\alpha_\infty - \alpha_0)$ ,  $n_\lambda$  and  $A_\lambda$  are model parameters obtained from experiments, and  $\alpha$  is the overall degree of reaction [DiLuzio & Cusatis 2013].

### 3.2 Age-dependent Lattice Discrete Particle Model

In 2011, Cusatis and coworkers developed the Lattice Discrete Particle Model (LDPM), a mesoscale discrete model that simulates the mechanical interaction of coarse aggregate pieces embedded in a cementitious matrix (mortar). The geometrical representation of the concrete mesostructure is constructed as follows: First, the coarse aggregate pieces, assumed to have spherical shapes, are introduced into the concrete volume randomly by a try-and-reject procedure. Secondly, nodes as zero-radius aggregate pieces are randomly distributed over the external surfaces to apply boundary conditions. Thirdly, based on Delaunay tetrahedralization, a three-dimensional domain tessellation creates a system of polyhedral cells interacting through triangular facets and a lattice system composed by the line segments connecting the aggregate centers.

LDPM has been utilized successfully to simulate concrete behavior under various loads [Cusatis 2011]. Furthermore it has been properly formulated to account for fiber reinforcement [Schauffert 2012] and has the ability to simulate the ballistic behavior of ultra-high performance concrete (UHPC) [Smith 2014]. In addition, LDPM showed success in structural scale analysis using multiscale methods [Cusatis 2014].

The concept of aging degree is used in the proposed aging model to account for early age phenomena. The individual material properties can be introduced as functions of the aging degree,  $\lambda$ , each capable of modifying part of the mechanical behavior. The proposed aging functions relating the local mesoscale material parameters with the aging degree are listed in Eq. 4 ~ 6. As seen, normal modulus, which is related to Young's modulus, has a linear relation with aging degree, by multiplying the asymptotic normal modulus  $E_0^\infty$ . Tensile strength, compressive strength, and transitional stress, on the other hand, have "power law" type relations with aging degree, by multiplying the corresponding asymptotes ( $\sigma_t^\infty$ ,  $\sigma_c^\infty$ ,  $\sigma_{N0}^\infty$ ). Last, the tensile characteristic length has a linear relation with aging degree, however rewritten to show the asymptotic tensile characteristic length,  $\ell_t^\infty$ , and that  $\ell_t$  decreases as concrete ages. Note, all the functions are structured such that when  $\lambda$  approaches the asymptotic value of 1 the corresponding parameters also approach their asymptotes.

The proposed aging functions for UHPC at early age with constants  $n_a$  and  $k_a$  are as follows:

$$E_0 = E_0^\infty * \lambda \quad (4)$$

$$\sigma = \sigma^\infty * \lambda^{n_a} \quad (5)$$

$$\ell_t = \ell_t^\infty (k_a(1 - \lambda) + 1) \quad (6)$$

## 4 LDPM modeling of UHPC: Calibration and Validation

The HTC model is calibrated by self desiccation RH measurements and validated by HR, HR+WB curing RH measurements. Also included in the output results of HTC are the simulated time history of cement hydration degree, silica fume reaction degree, total reaction degree, and overall aging degree calculated by Eq. 3.

The HTC input data include boundary conditions and material properties. The environmental boundary conditions are as follows: for HR curing: 22°C and 100% RH for 14 days then 50% RH afterwards; for HR+WB curing: 22°C and 100% RH for 7 days, then 85°C and 100% RH for the next 7 days and afterwards 50% RH at room temperature; and for self desiccation curing: sealed and room temperature.

The calibrated and validated HTC model provides the spatial distribution of the aging degree which serves as input for the aging functions defining the local mesoscale mechanical properties of LDPM. The aging functions, Eq. 4 ~ 6, are formulated in such a way as to capture the aging mechanical properties with the simplest possible functional relationship and hence the lowest number of parameters that need to be calibrated. The aging mechanical properties are captured by the mesoscale model parameters: normal modulus, tensile strength, stress at pore collapse, transitional stress, and tensile characteristic length.

For the UHPC in this study a good agreement between experiments and simulations are obtained by setting  $n_a = 2.33$ , and  $k_a = 22.2$ , for the aging functions. All the LDPM simulations utilize a coarse aggregate size 2 ~ 4 mm in order to save computational cost.

Generally speaking, the model is calibrated first by TPB (notched) and cylinder compression test results and later validated by the other types of tests including circular disk Brazilian, cube compression, unnotched beam bending, as well as size effect tests. Averaged experimental data as well as simulation results of beam 3-point-bending (50% notched) for different ages can be found in Fig. 1 [Wan 2015], where the nominal flexural stress is obtained by equation  $\sigma_N = 3PS/2BH^2$  ( $[3 \times \text{load} \times \text{test span}] / [2 \times \text{specimen depth} \times \text{specimen height}^2]$ ) and nominal strain by  $\epsilon_N = \text{CMOD} / \text{specimen height}$ . The strength gain and stress-strain curve shapes from simulations match those from experiments quite well. As the UHPC ages, its strength increases while ductility decreases.

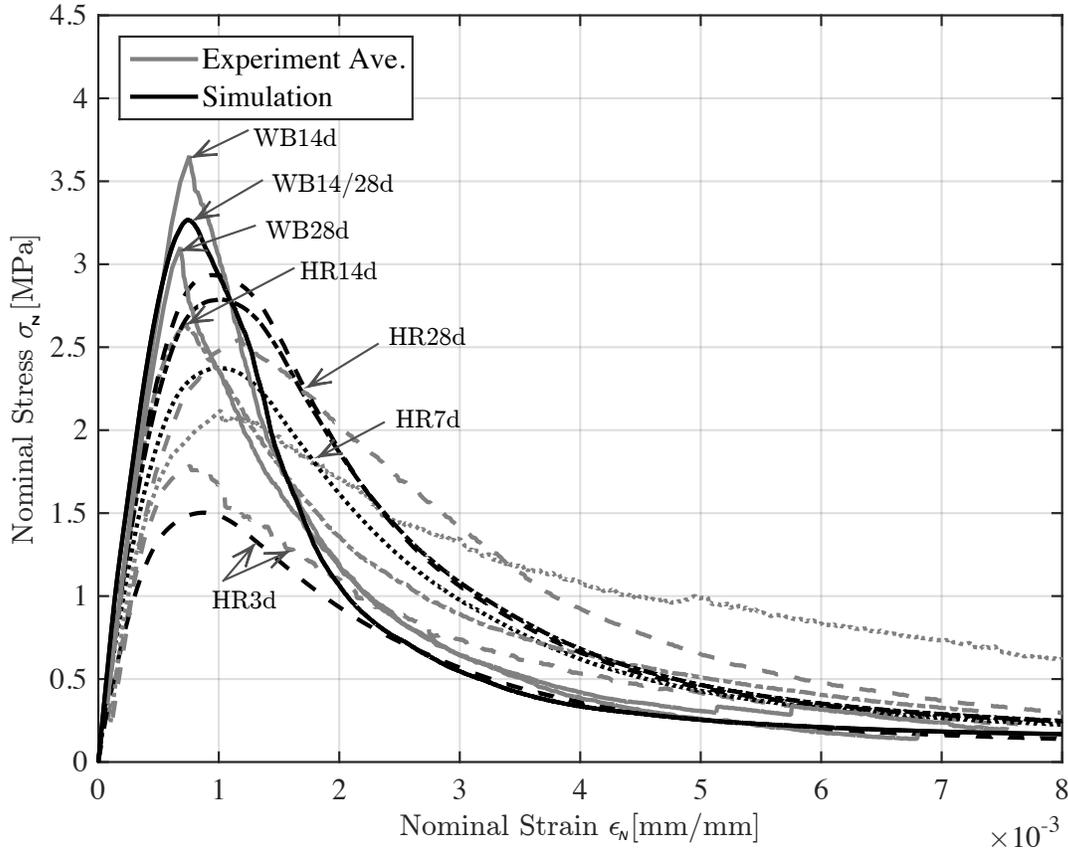


Figure 1: LDPM Simulations for 3-point-bend Test

## 5 UHPC Size effect Study

Three sizes of beams were cast with a geometrical scaling factor of  $\sqrt{5}$  for height & span with constant thickness of 1" (25.4 mm), of which the nominal dimensions are listed in Table 1. Height to span ratio is kept as 1:4. The same as of the previous early age specimens, curing routine of 7 days in 100% humidity room (HR) then 7 days in hot water bath at 85 °C (HR + WB) was followed. After in total of 14 days HR+WB curing, the specimens were stored at room temperature and average RH of 50% until testing. Aged 120 days on average, the specimens were cut to have 50% notch depth, and were tested with TPB configuration in CMOD control. The test results are shown in Fig. 2. The total fracture energy  $G_F$ , is calculated according to the work of fracture method, as the area under the force-displacement curves.

The LDPM simulation results, as pure prediction, for each size can be found in Fig. 2, where experimental statistics are also included. More than three specimens with different particle placement were utilized for size L and XL simulations respectively to show the scatter for large sizes. Overall, the simulations can represent the UHPC behavior under TPB test with very high accuracy and capture the experimentally observed size effect for fully cured specimens. The crack patterns from simulations also coincide with those of the TPB experiments. Thus, it can be assumed that the model can also predict well the age

Table 1: Nominal specimen dimensions for size effect investigation

Size	Length $L$ [mm]	Thickness $B$ [mm]	Height $H$ [mm]	Test Span $S$ [mm]
M	127	25.4	25.4	101.6
L	254	25.4	56.8	227.2
XL	558.8	25.4	127	508

dependence of size effect.

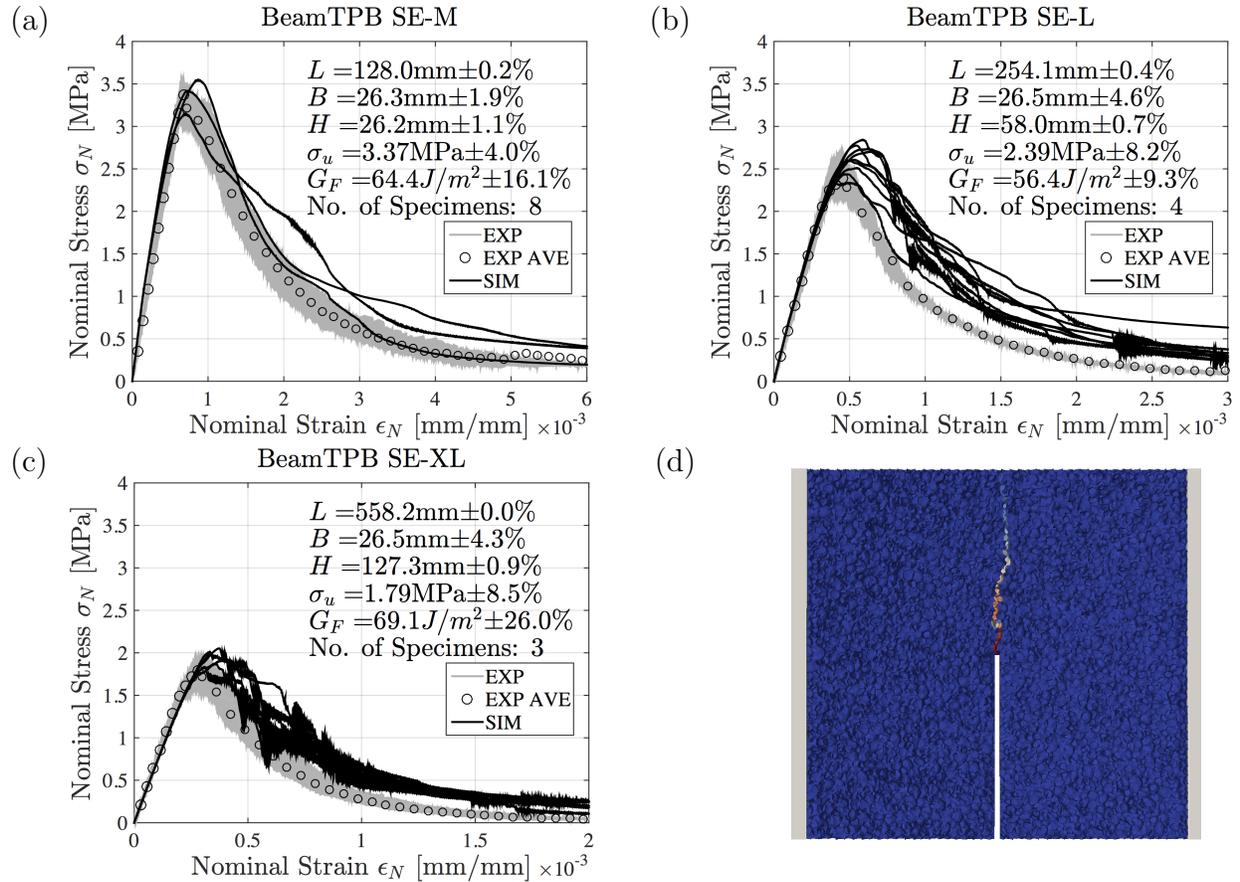


Figure 2: UHPC size effect experiments vs. LDPM simulations for (a) size M (b) size L (c) size XL and (d) simulated crack propagation for size XL

## 6 Conclusion

This paper describes a LDPM-based hygro-thermo-chemo-mechanical early age model, for UHPC, calibrated and validated by relative humidity measurements and experimental mechanical test data. By coupling the HTC model and the LDPM, the development of the internal structure of the cement phase, its effects on mechanical properties, as well as size effect

can be accurately and comprehensively captured by the proposed computational framework. The aging functions developed as a bridge between HTC and LDPM have great simplicity and easy applicability.

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