EXPERIMENTAL AND COMPUTATIONAL ANALYSIS OF THE BEHAVIOR OF ULTRA HIGH PERFORMANCE CONCRETE AT EARLY AGE

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Abstract:

Ultra high performance concretes (UHPCs) are cementitious composite materials with high level of performance characterized by high compressive strength, high tensile strength and superior durability, reached by low water-to-binder ratio, optimized aggregate size distribution, thermal activation, and fiber reinforcement. In the past couple of decades, more and more UHPCs have been developed and found their way into practice. Thus, also the demand for computational models capable of describing and predicting relevant aging phenomena to assist design and planning is increasing. This paper presents the early age experimental characterization as well as the results of subsequent simulations of a typical UHPC matrix. Performed and simulated tests include unconfined compression, splitting (Brazilian), and three-point-bending tests. The computational framework is formulated by coupling a hygro-thermo-chemical (HTC) theory with a comprehensive mesoscale discrete model. The HTC component allows taking into account various types of curing conditions with varying temperature and relative humidity and predicting the level of concrete aging, while the mechanical component, based on a recently formulated discrete model, the Lattice Discrete Particle Model (LDPM), permits the simulation of the failure behavior of concrete at the length scale of major heterogeneities. The obtained results provide both insight in UHPC early age mechanisms and a computational model for the analysis of aging UHPC structures.

1 Introduction

Ultra high performance concretes (UHPCs) are cementitious composites characterized by high compressive strength, typically greater than 150 MPa (21.7 ksi), low water-binder ratio, optimized gradation curve, use of thermal activation, fiber reinforcement and superplasticizers. Moreover, UHPC has a discontinuous pore structure that reduces liquid ingress and permeability, which leads to significantly enhanced durability, longer service life and lower costs for maintenance. UHPC became commercially available in the beginning of the 21st century and has been utilized in the construction industry especially for bridge applications and tall buildings around the world across North America, Europe, and Asia.

Among various types of UHPCs developed by researchers around the world, Ductal is the most commonly used and commercially available in the United States, Europe and Asia. Other types of UHPCs include but are not limited to compact reinforced composite (CRC) developed by Aalborg Portland in 1986, the UHPC mix
of Teichmann and Schmidt in Germany, and CorTuf developed by the U.S. Army Corps of Engineers Research and Development Center (ERDC), which all utilize water/cement ratio within the range of 0.15∼0.21, fine aggregate gradation, superplasticizers and steel fibers [44].

With the increased adoption of UHPC materials in practice, also increasing is the demand for computational models that can be utilized in design. For example, Chen and Graybeal [35] investigated the behavior of existing UHPC structural components including prestressed 'I' and 'pi' shaped girders by finite element methods with good abilities of replicating the structural response. However, conventional constitutive formulations are unable to capture the evolution of material properties and correspondingly the time-dependent structural response of concrete as an aging material. This is an important aspect to consider given that the current construction practice requires shorter and shorter construction times associated with, for example, early load applications and prestressing. While the contributions of fibers are quintessential for the success of UHPCs, their contribution can be assumed to be non-aging. In this paper we focus on the evolution of the matrix properties.

It is well known that the strength of cement based composites such as concrete increases rapidly at early age. However, the chemical and physical mechanisms behind this phenomenon are complex and consist of multiple coupled components. The cross-effects between hydration reaction, temperature evolution, and member deformation involve complex chemo-physical mechanisms that operate over a broad range of length and time scales, from nanometer to meter [14], and from fractions of seconds to years. Notably, evolution laws for maturing concrete based on Arrhenius-type time acceleration concepts are widely supported by a good agreement with experimental data [3, 4, 7].

Ulm and Coussy [7] studied the thermo-chemo-mechanical coupling of concrete at early age with a formulation based upon thermodynamics of open porous media composed of a skeleton and several fluid phases saturating the porous space. It accounts explicitly for the hydration of cement by considering the thermodynamic imbalance between the chemical constituents in the constitutive modeling at the macrolevel of material description. However, the effects from stress and temperature evolutions were neglected. Afterwards they extended the thermo-chemo-mechanical cross effects characterizing the autogeneous shrinkage, hydration heat and strength growth, within the framework of chemoplasticity [14]. Cervera et. al. [15] applied the reactive porous media theory and introduced a novel aging model which accounts for the effect of curing temperature evolution featuring the aging degree as an internal variable. They proposed that the evolution of the compressive
and tensile strengths and elastic moduli can be predicted in terms of the evolution of the aging degree [17, 18]. The model considers the short-term mechanical behavior based on the continuum damage mechanics theory and the long-term mechanical behavior based upon the microprestress-solidification theory [16]. Bernard, Ulm and Lemarchand [20] developed a multi scale micromechanics-hydration model to predict the aging elasticity of cement-based materials starting at the nano level of the C-S-H matrix. Lackner and Mang [24] proposed a 3-D material model for the simulation of early-age cracking of concrete based on the Rankine criterion formulated in the framework of multi surface chemoplasticity. Gawin, Pesavento, and Schrefler [26, 27] proposed a solidification-type early-age model and extended it to account for coupled hygro-thermo-chemo-mechanical phenomena, which was applied to solving practical problems, such as reparation and analysis of concrete structures [47, 50].

Di Luzio and Cusatis [33, 34] formulated, calibrated, and validated a hygro-thermo-chemical (HTC) model suitable for the analysis of moisture transport and heat transfer for standard as well as high performance concrete. In this study, classical macroscopic mass and energy conservation laws were formulated in terms of 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 [33]. Furthermore, Di Luzio and Cusatis [45], amalgamated the microplane model [29, 30, 31] and the microprestress-solidification theory. This unified model takes into account all the most significant aspects of concrete behavior, such as creep, shrinkage, thermal deformation, and cracking starting from the initial stages of curing up to several years of age.

While continuum mechanics and finite element solvers are broadly utilized for mechanical analysis of concrete structures at the macroscopic levels, the Lattice Discrete Particle Model (LDPM) [38, 39] provides additional insights into failure behavior of concrete at smaller length scales. 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 [38].

The HTC model and LDPM are selected as basis for the early age mechanical model formulated in this study. On one hand, the HTC model can comprehensively capture the hygral and thermal evolutions and chemical reactions during aging, and on the other hand, LDPM can provide insights into the concrete behavior on the mesoscale level and also simulate well the mechanical behavior of concrete structures under various loads on the macroscopic level. The two models are connected by a set of proposed aging functions that form the core
of the proposed HTC-LDPM coupled early age framework that now allows to accurately predict the behavior of concrete members at early age and beyond.

2 Computational Framework for the Simulation of UHPC at Early Age

The proposed hygro-thermo-chemo-mechanical early-age model for cement based concrete consists of two major components: the HTC model and the LDPM with aging material properties.

2.1 Hygro-Thermo-Chemical (HTC) model

The behavior of concrete at early age heavily depends on moisture content and temperature. The overall moisture transport can be described through Fick’s law that expresses the flux of water mass per unit time $J$ as a function of the spatial gradient of the relative humidity $h$. Moisture mass balance requires the variation in time of the water mass per unit volume of concrete to be equal to the divergence of moisture flux $J$. 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 $w_n$ [1, 2, 6]. 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 $w_e = w_e(h, \alpha_c, \alpha_s)$, which represents an age-dependent sorption/desorption isotherm. Consequently, the moisture mass balance equation reads [33]:

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

The enthalpy balance is also influenced by the chemical reactions occurring at the early age. One can write, at least for temperatures not exceeding 100 °C [8],

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

where $\dot{Q}_c^\infty =$ hydration enthalpy, $\dot{Q}_s^\infty =$ latent heat of silica-fume reaction per unit mass of reacted silica-fume, $\rho$ is the mass density of concrete, $\lambda$ is the heat conductivity, and $c_t$ is the isobaric heat capacity of concrete.

According to the thermodynamics based model proposed by Ulm and Coussy [7, 25] and later revised by...
Cervera et al. [15], the hydration kinetics can be described by postulating the existence of a Gibb’s free energy dependent on the external temperature \( T \) and the hydration extent \( \chi_c \). For convenience the hydration degree can be defined as \( \alpha_c = \chi_c / \chi_c^\infty \), where \( \chi_c^\infty \) is the theoretical asymptotic value of the hydration extent in ideal hygrometric conditions. Analogously, the asymptotic degree of hydration, can be expressed as \( \alpha_c^\infty = \chi_c^\infty / \chi_c^\infty \).

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 though the layer of cement hydrates is an exponential function of the hydration extent [7], Cervera et al. [15] proposed the evolution equation for the hydration degree:

\[
\dot{\alpha}_c = A_c(\alpha_c) e^{-E_{ac}/RT},
\]

where \( A_c(\alpha_c) \) is the normalized chemical affinity, \( E_{ac} \) is the hydration activation energy, \( R \) is the universal gas constant, and \( \eta, A_{c1}, \) and \( A_{c2} \) are material parameters. To account for the situation that the hydration process slows down and may even stop if the relative humidity decreases below a certain value, 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 Bažant and Prasannan [5]. 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 [5, 26].

The theory adopted for cement hydration can be as well utilized for silica fume (SF) reaction since the kinetics of pozzolanic reaction can also be assumed to be diffusion controlled. Accordingly, the degree of SF reaction, \( \alpha_s \) is introduced [33],

\[
\dot{\alpha}_s = A_s(\alpha_s) e^{-E_{as}/RT},
\]

and \( A_s(\alpha_s) = A_{s1}(\frac{\alpha_s^\infty}{\alpha_s^\infty} + \alpha_s)(\alpha_s^\infty - \alpha_s) e^{-\eta_s \alpha_s/\alpha_s^\infty}, \)

where \( A_s \) is the SF normalized affinity, \( E_{as} \) is the activation energy of SF reaction, and \( \alpha_s^\infty \) is the asymptotic value of the SF reaction degree. \( E_{as}/R = 9700K \) can be generally assumed [11]. The rate of SF reaction degree is assumed not to depend on \( h \).

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. ambient relative humidity and especially curing temperature [12, 17, 19]. To account for this additional effect the aging degree \( \lambda \) is typically used and formulated as:

\[
\dot{\lambda} = \left( \frac{T_{max} - T}{T_{max} - T_{ref}} \right)^{n\lambda} (B_\lambda - 2A_\lambda \alpha) \tag{3}
\]

where \( B_\lambda = [1 + A_\lambda(\alpha_s^\infty - \alpha_s^0)]/\alpha_s^\infty - \alpha_s^0 \), \( n_\lambda \) and \( A_\lambda \) are model parameters obtained from fitting experimental
data, and $\alpha$ is the overall degree of reaction defined as [45]

$$\alpha(t) = \frac{\alpha_c(t)c^\infty + \alpha_s(t)s^\infty}{c^\infty + s^\infty}$$

(4)

2.2 Age-dependent Lattice Discrete Particle Model

In 2011, Cusatis and coworkers [38, 39] 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 concrete mesostructure is constructed through the following steps. First, the coarse aggregate pieces, assumed to have spherical shapes, are introduced into the concrete volume by a try-and-reject random procedure. Secondly, nodes as zero-radius aggregate pieces are randomly distributed over the external surfaces to facilitate the application of boundary conditions. Thirdly, a three-dimensional domain tessellation, based on the Delaunay tetrahedralization of the generated particle centers, creates a system of polyhedral cells (see Fig. 1) interacting through triangular facets and a lattice system composed by the line segments connecting the aggregate centers. The full description of LDPM geometry is reported in Ref [38, 39].

![Figure 1: One LDPM Cell around an aggregate piece.](image)

In LDPM, rigid body kinematics is used to describe the deformation of the lattice particle system and the displacement jump, $[u_C]$, at the centroid of each facet is used to define measures of strain as

$$e_N = \frac{n^T[u_C]}{\ell}; \quad e_L = \frac{l^T[u_C]}{\ell}; \quad e_M = \frac{m^T[u_C]}{\ell}$$

(5)

where $\ell =$ interparticle distance; and $n$, $l$, and $m$, are unit vectors defining a local system of reference attached to each facet. It was recently demonstrated that the strain definitions in Eq. 5 correspond to the projection into the local system of references of the strain tensor typical of continuum mechanics [37, 46, 49].
Next, a vectorial constitutive law governing the behavior of the material is imposed at the centroid of each facet. In the elastic regime, the normal and shear stresses are proportional to the corresponding strains:

\[ t_N = E_N e_N^* = E_N (e_N - e_N^0); \quad t_M = E_T e_M^* = E_T (e_M - e_M^0); \quad t_L = E_T e_L^* = E_T (e_L - e_L^0), \]

where \( E_N = E_0, \) \( E_T = \alpha E_0, \) \( E_0 = \) effective normal modulus, and \( \alpha = \) shear-normal coupling parameter; and \( e_N^0, e_M^0, e_L^0 \) are mesoscale eigenstrains that might arise from a variety of phenomena such as, but not limited to, thermal expansion, creep, shrinkage, and chemical reactions, e.g., alkali-silica reaction.

For stresses and strains beyond the elastic limit, the LDPM formulation considers the following nonlinear mesoscale phenomena [21, 22, 38]: (1) fracture and cohesion; (2) compaction and pore collapse; and (3) friction.

**Fracture and cohesion due to tension and tension-shear.** For tensile loading \((e_N^* > 0)\), the fracturing behavior is formulated through an effective strain, \( e^* = \sqrt{e_N^2 + \alpha (e_M^2 + e_L^2)} \), and stress, \( t = \sqrt{t_N^2 + (t_M + t_L)^2}/\alpha \), which define the normal and shear stresses as \( t_N = e_N^*(t/e^*); t_M = \alpha e_M^*(t/e^*); t_L = \alpha e_L^*(t/e^*) \). The effective stress \( t \) is incrementally elastic \((t = E_0 \dot{e})\) and must satisfy the inequality \( 0 \leq t \leq \sigma_{bf}(e, \omega) \) where \( \sigma_{bf} = \sigma_0(\omega) \exp [-H_0(\omega)(e - e_0(\omega))/\sigma_0(\omega)] \), \( x = \max\{x, 0\} \), and \( \tan(\omega) = e_N^*/\sqrt{\alpha e_T^*} = t_N \sqrt{\alpha}/t_T \), and \( e_T^* = \sqrt{e_M^2 + e_L^2} \). The post peak softening modulus is defined as \( H_0(\omega) = H_t(2\omega/\pi)^n \), where \( H_t \) is the softening modulus in pure tension \((\omega = \pi/2)\) expressed as \( H_t = 2E_0/(\ell_t/\ell - 1); \ell_t = 2E_0G_t/\sigma_t^2 \); \( \ell \) is the length of the tetrahedron edge; and \( G_t \) is the mesoscale fracture energy. LDPM provides a smooth transition between pure tension and pure shear \((\omega = 0)\) with parabolic variation for strength given by \( \sigma_0(\omega) = \sigma_t r_{st}^2 \left[-\sin(\omega) + \sqrt{\sin^2(\omega) + 4\alpha \cos^2(\omega)}/r_{st}^2 \right]/[2\alpha \cos^2(\omega)] \), where \( r_{st} = \sigma_s/\sigma_t \) is the ratio of shear strength to tensile strength.

**Compaction and pore collapse from compression.** Normal stresses for compressive loading \((e_N^* < 0)\) must satisfy the inequality \(-\sigma_{bc}(e_D, e_V) \leq t_N \leq 0 \), where \( \sigma_{bc} \) is a strain-dependent boundary depending on the volumetric strain, \( e_V \), and the deviatoric strain, \( e_D = e_N - e_V \). The volumetric strain is computed by the volume variation of the Delaunay tetrahedra as \( e_V = \Delta V/3V_0 \) and is assumed to be the same for all facets belonging to a given tetrahedron. Beyond the elastic limit, \(-\sigma_{bc} \) models pore collapse as a linear evolution of stress for increasing volumetric strain with stiffness \( H_c \) for \(-e_V \leq e_{c1} = \kappa_{c0} e_{c0} \): \( \sigma_{bc} = \sigma_{c0} + (-e_V - e_{c0}) H_c(r_{DV}); H_c(r_{DV}) = H_{c0}/(1 + \kappa_{c2} (r_{DV} - \kappa_{c1})); \sigma_{c0} \) is the mesoscale compressive yield stress; \( r_{DV} = e_D/e_V \) and \( \kappa_{c1}, \kappa_{c2} \) are material parameters. Compaction and rehardening occur beyond pore collapse \((-e_V \geq e_{c1}) \). In this
case one has \( \sigma_{bc} = \sigma_{c1}(r_{DV}) \exp \left[ (-e_V - e_{c1})H_c(r_{DV})/\sigma_{c1}(r_{DV}) \right] \) and \( \sigma_{c1}(r_{DV}) = \sigma_{c0} + (e_{c1} - e_{c0})H_c(r_{DV}). \)

**Friction due to compression-shear.** The incremental shear stresses are computed as \( \dot{t}_M = E_T(\dot{e}^*_M - \dot{e}^{*p}_M) \) and \( \dot{t}_L = E_T(\dot{e}^*_L - \dot{e}^{*p}_L) \), where \( \dot{e}^{*p}_M = \xi \partial \varphi / \partial t_M \), \( \dot{e}^{*p}_L = \dot{\xi} \partial \varphi / \partial t_L \), and \( \xi \) is the plastic multiplier with loading-unloading conditions \( \varphi \dot{\xi} \leq 0 \) and \( \dot{\xi} \geq 0 \). The plastic potential is defined as \( \varphi = \sqrt{t^2_M + t^2_L - \sigma_{bs}(t_N)} \), where the nonlinear frictional law for the shear strength is assumed to be \( \sigma_{bs} = \sigma_s + (\mu_0 - \mu_\infty)\sigma_{N0}\left[1-\exp(t_N/\sigma_{N0})\right]-\mu_\infty t_N \); \( \sigma_{N0} \) is the transitional normal stress; \( \mu_0 \) and \( \mu_\infty \) are the initial and final internal friction coefficients.

Each material property in LDPM governs part of the concrete behavior under loading. The normal elastic modulus, which refers to the stiffness for the normal facet behavior, \( E_0 \), governs LDPM response in the elastic regime, along with the coupling parameter \( \alpha \). Approximately, the macro scale Young's modulus \( E \) and Poisson’s ratios \( \nu \) can be calculated as \( E = E_0(2 + 3\alpha)/(4 + \alpha) \) and \( \nu = (1 - \alpha)/(4 + \alpha) \). Typical concrete Poisson’s ratio of about 0.18 is obtained by setting \( \alpha = 0.25 \) [39].

The tensile strength, \( \sigma_t \), and characteristic length, \( \ell_t \), together define the softening behavior due to fracture in tension of LDPM facets [39], with the relation \( G_t = \ell_t\sigma^2_t/2E_0 \), where \( G_t \) is the mesoscale fracture energy. Calibration of \( \sigma_t \) and \( \ell_t \) is typically achieved by fitting experimental data, e.g. the load-displacement curve of a three-point-bending test.

The softenig exponent, \( n_t \), governs the interaction between shear and tensile behavior during softening at the facet level. One obtains more ductile behavior in both compression and tension by increasing \( n_t \), however the increase is more pronounced in compression than in tension. The shear strength, \( \sigma_s \), is the facet strength for pure shear and affects the macroscopic behavior in unconfined compression. Yielding compressive stress, \( \sigma_{c0} \), initial hardening modulus, \( H_{c0} \), transitional strain ratio, \( k_{c0} \), and densified normal modulus, \( E_d \), define the behavior of the facet normal component under compression and affect mostly the macroscopic behavior in hydrostatic and highly-confined compression. The initial internal friction, \( \mu_0 \), and transitional stress, \( \sigma_{N0} \), mainly govern the mechanical response in compression and have no influence on tensile behavior in LDPM. At the macroscopic level they mostly affect compressive behavior at zero or low confinement. Descriptions of effects and functions of other LDPM mesoscale parameters can be found in Cusatis et. al. [39].

Besides the compatibility and constitutive equations discussed above, the governing equations of the LDPM framework are completed through the equilibrium equations of each individual particle.

LDPM has been utilized successfully to simulate concrete behavior under various loading conditions [38, 39].
Furthermore, the framework has been extended to properly account for fiber reinforcement [41, 42] and has the ability to simulate the ballistic behavior of ultra-high performance concrete (UHPC) [48]. In addition, LDPM showed success in structural scale analysis using multiscale methods [46, 40, 51].

The concept of aging degree is applied in the proposed early age model to quantify maturity of concrete. Mesoscale material properties, which govern the mesoscale constitutive equations, change while concrete ages and can be formulated as functions of the aging degree. For example, Karte et al. [52] and Chamrova [36] found that unloading modulus $E$ increases linearly in terms of cement hydration degree. While Schutter and Taerwe [9] observed a nonlinear relation between Young’s modulus and degree of hydration, for different mixes.

The proposed aging functions relating the mesoscale material parameters with aging degree are listed in Eq. $6 \sim 8$. As seen, the normal modulus, $E_0$, which is related to the elastic modulus, is assumed to have a linear relation with aging degree $\lambda$. Tensile strength, $\sigma_t$, compressive yielding stress, $\sigma_c$, and transitional stress, $\sigma_{N0}$, on the other hand, are assumed to have power-law type relations with aging degree. Lastly, the tensile characteristic length, $\ell_t$, is assumed to be a linear decreasing function with aging degree, to simulate the well known brittleness increase with age. All the aging functions are formulated such that the corresponding parameters approach their asymptotic values for $\lambda$ approaching the value of 1.

The proposed aging functions for UHPC at early age read

$$E_0 = E_0^\infty \lambda$$  

$$\sigma_t = \sigma_t^\infty \lambda^{n_a}; \, \sigma_c = \sigma_c^\infty \lambda^{n_a}; \, \sigma_{N0} = \sigma_{N0}^\infty \lambda^{n_a}$$  

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

where $n_a$ and $k_a$ are positive constants. The other LDPM mesoscale parameters, are assumed age-independent due to a lack of relevant experimental data on the response in compression under confinement.

3 Experimental Characterization of Early Age Behavior of UHPC

In order to calibrate and validate the proposed early age model, an experimental campaign was carried out to
characterize the early age mechanical behavior of a UHPC. The mixture proportions for the adopted mix design are reported below in Table 1. The material composition consists of LaFarge Type H cement, F-50 Ottawa 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, which is a foundry grade Ottawa sand [32].

| Ingredient     | Type               | Proportion | Weight per kg |
|----------------|--------------------|------------|---------------|
| Cement         | Lafarge Type H     | 1.0000     | 0.3497        |
| Sand           | F-50               | 0.9674     | 0.3383        |
| Silica Flour   | Sil-co-sil 75      | 0.2768     | 0.0968        |
| Silica Fumes   | Elkem ES-900W      | 0.3890     | 0.1360        |
| Superplasticizer | ADVA-190      | 0.0180     | 0.0063        |
| Water          | Tap Water          | 0.2082     | 0.0728        |

The baseline curing regime for the adopted UHPC [32] consisted of casting on day 0, demolding on day 1, curing in 100% humidity room (HR) with room temperature of approximately 23°C until day 7, followed by curing for 4 days in 85°C water bath (WB), and 2 days drying in the oven at 85°C. Preliminary unconfined compression tests using 2×4 in (50.8×101.6 mm) cylinders were carried out at nominal ages of 1 day, 7 days, 11 days and 13 days. At least 3 specimens were tested for each age to obtain average and standard deviation values. Measured compressive strength for the 4 different ages were 13 MPa ± 31%, 66 MPa ± 23%, 123 MPa ± 29%, and 120 MPa ± 21%. As seen from the results, the oven curing does not provide an increase in compressive strength, and actually, a slight decrease of 2%, was observed. Consequently, later experiments disregarded the oven curing procedure.

To study the effects of hot water bath curing on strength gain, two curing protocols with and without hot water bath curing were explored. A first group of specimens was kept in the humidity room (HR) for 14 days, a second group, instead, was kept in the humidity room for 7 days after which it was placed in hot water bath (WB) at 85°C for another 7 days. Both groups were later exposed to the same laboratory conditions (about 22 °C and 50% RH). Unconfined compression tests using 2×2 in (50.8×50.8 mm) cylinders, three-point-bending (TPB) tests with half-depth notched 1×1×5 in (25.4×25.4×127 mm) beams, and tensile splitting tests using 3×1 in (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 CMOD opening control for three-point bending and splitting tests were utilized to avoid brittle failure and to obtain full post-peak information. Furthermore, a friction reducing layer (moly dry lubricant) was applied to the load platens in compression tests.
3.1 Unconfined Cylinder Compression Test

Unconfined compression tests were performed in a closed loop servo-hydraulic MTS load frame with a maximum capacity of 4.4 MN (1000 kips). A circumferential extensometer was utilized to control expansion of the specimens with the goal to obtain post-peak response (see Fig. 2a).

In order to ensure consistent and accurate test results, a Standard Operation Procedure (SOP) for testing was created and followed. The specimen data sheet, or protocol, was filled out with Vernier Calliper measurements of diameter and height (average of 4 measurements for each dimension), control mode, loading rate and time of loading. After centering the specimen, a preload of 1-5% of the expected peak was applied before the actual test commenced.

For compression tests, two phases of control were used: first stroke control followed by circumferential expansion control. Both control modes applied a loading rate of 0.001 mm/s. The mode of control was switched at estimated 30% of the potential peak load. Compression test results can be found in Table 2 and Figure 10, where stress is calculated as $\sigma = P/A$ (load/area) and strain as $\varepsilon = \Delta d/H$ (relative displacement between loading platens/specimen height). Geometry measurements of height $H$ and diameter $D$ with standard deviations are also shown in the figures.

As Table 2 shows, at 14 days, samples that were cured in hot water bath had about 28% more strength compared with the steam cured. However, after 14 more days in air (from day 14 to day 28) the strength gain was almost completely lost and the water cured samples were only 1% stronger than the others. This effect was, most likely, the result of both cooling and shrinkage cracking.
### Table 2. Unconfined Cylinder Compression Test Results

| Nominal Age [d] | Actual Ave. Age [d] | Curing | Strength [MPa] | No. of Specimens |
|-----------------|---------------------|--------|----------------|------------------|
| 3               | 2.9                 | HR     | 53.8           | 4                |
| 7               | 7.0                 | HR     | 78.4           | 4                |
| 14              | 14.5                | HR     | 99.3           | 4                |
| 28              | 29.8                | HR     | 115.6          | 3                |
| 14              | 14.4                | HR + WB| 127.2          | 4                |
| 28              | 30.0                | HR + WB| 116.7          | 5                |

### 3.2 Brazilian Test

Indirect tensile splitting (Brazilian) tests were performed in a MTS load frame with a maximum axial capacity of 220,000 lbs (about 1 MN). The testing procedure was developed according to ASTM C496. Loading blocks with dimensions of 0.6 × 1.5 × 6.25 in (15 × 38 × 159 mm) were used. Initially, localized failure in compression was avoided by the utilization of wooden support strips, however, their usage introduced an unwanted compliance at the beginning of the test. Therefore, aging tests had been ran without wooden strips. Contrary to ASTM C496 which calls for standard cylinder dimensions of e.g. 2 × 4 in (50.8 × 101.6 mm), cylindrical disks of 3” (76.2 mm) in diameter and 1” (25.4 mm) in thickness were tested (see Fig. 2b). This specimen geometry allows a relatively more stable transition to the post-peak regime and consistent tensile strain readings.

Similar to compression tests, a standard operating procedure for splitting tests was developed and followed. After the specimen was placed firmly in the MTS Load Frame and preloaded with approximately 1 % of estimated peak to ensure contact between specimen and loading supports, the first phase of the actual test was carried out in load control with a loading rate of 0.1 kN/sec. As soon as 50 % of the estimated peak was reached, the test was switched to crack mouth opening displacement (CMOD) control to save experiment time and avoid sudden failure. A relatively stable CMOD rate was found to be 5 × 10^{-7} mm/sec for the highly brittle UHPC specimens. After reaching a stable response in CMOD control, the opening rate could be manually adjusted and accelerated to save testing time while ensuring stability. Although at least 3 specimens were prepared for testing on each age and great precautions were taken, many of the specimens still exhibited brittle failure and thus full post-peak behavior could not be captured. Brazilian test results, including age of concrete at testing, curing conditions, nominal strength, number of specimens and dimension measurements, are shown in Table 3.

The nominal tensile splitting strength is computed as \( \sigma_u = \frac{2P}{\pi hd} \left( \frac{[2 \times \text{load}]}{[\pi \times \text{height} \times \text{diameter}]} \right) \). Partly due to the inconsistent loading rates, which were controlled by manual switch for the tests on different ages,
the tensile strength does not quite follow the expected aging trend.

Table 3. Brazilian Test Results

| Nominal Age | Actual Ave. Age | Curing | Splitting Tensile Strength [MPa] | Number of Specimens | Diameter d [mm] | Height h [mm] |
|-------------|-----------------|--------|--------------------------------|---------------------|----------------|--------------|
| 3           | 3.0             | HR     | 4.5                            | 3                   | 76.3 ± 0.3%    | 23.2 ± 9.0%  |
| 7           | 7.0             | HR     | 5.2                            | 3                   | 76.3 ± 0.2%    | 24.5 ± 4.0%  |
| 14          | 14.9            | HR     | 5.5                            | 1                   | 76.4 ± 0.0%    | 23.3± 0.0%   |
| 28          | 29.6            | HR     | 4.5                            | 3                   | 76.2 ± 0.3%    | 24.5± 4.5%   |
| 14          | 14.6            | HR + WB| 11.4                           | 3                   | 76.3 ± 0.3%    | 25.4 ± 10.4% |
| 28          | 29.2            | HR + WB| 9.4                            | 3                   | 76.4± 0.2%     | 24.7 ± 3.3%  |

3.3 Three-point-bending Fracture Test

Beam specimens with 1×1×5 in (25.4×25.4×127 mm) dimensions were cast for TPB tests (see Fig. 2c), with notches of 50 % relative depth. The nominal span (distance between bottom supports) was 4 in (101.6 mm). An extensometer sensor was glued to the bottom of the specimen with the notch between its two feet. After a pre-load of up to 5% of the expected peak was applied, the specimen was loaded in CMOD control with an initial loading rate of 0.0001 mm/sec. This rate could be increased in the late post-peak phase to save total testing time while ensuring a fully recorded softening behavior. The test results and nominal stress-strain curves can be found in Table 4 and Fig. 9, where the nominal flexural stress is obtained by equation \( \sigma = \frac{3PS}{2BH^2} \) \(([3\times \text{load} \times \text{test span}]/[2\times \text{specimen width} \times \text{specimen depth}^2])\) and nominal strain by \( \epsilon = \frac{\text{CMOD}}{\text{specimen depth}} \), the total fracture energy \( G_F \) is calculated as the area under the force-displacement curve divided by the ligament area. Geometry measurement statistics are also included in the figures.

Table 4. Three-point-bending Test Results

| Nominal Age [d] | Actual Ave. Age [d] | Curing       | Max. Nominal Stress [MPa] | No. of Specimens |
|-----------------|---------------------|--------------|---------------------------|-----------------|
| 3               | 2.9                 | HR           | 1.79                      | 3               |
| 7               | 7.0                 | HR           | 2.12                      | 3               |
| 14              | 14.0                | HR           | 2.65                      | 4               |
| 28              | 28.0                | HR           | 2.55                      | 4               |
| 14              | 14.4                | HR + WB      | 3.65                      | 4               |
| 28              | 28.0                | HR + WB      | 3.10                      | 4               |

As observed from the experimental results of all types of mechanical testing, in general, the material exhibits an increasing trend in strength as it ages. However, the strengths decrease from 14 days to 28 days for all tests and curing conditions, except compression HR, when the specimens were stored in air, potentially causing
drying shrinkage damage which leads to strength decrease.

3.4 Relative Humidity Measurements

In order to calibrate the HTC model for the UHPC, which can later provide the spatial fields of relative humidity, temperature, and reaction/aging degrees needed for the mechanical analysis, RH measurements at the center of the specimens as well as at the specimen boundaries (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. For each curing method, five 2x2 in (50.8×50.8 mm) cylinders were measured by RH&T sensors, see Fig. 3. At the time of casting, a straw with one side closed by nylon mesh screens and housing a RH&T sensor, was vertically inserted into each specimen with the perforated end centered in the specimen. The other end of the straw outside each specimen was sealed with moisture-tight silicone sealant. The RH&T sensors remained in the self-desiccation specimens for the whole measurement period, which were sealed with plastic molds (Fig. 3-c), silicone sealant and plastic films. For the unsealed samples, during and after 100% RH humidity room curing, the RH&T sensors were taken out and put back in about once a day to avoid condensation while the operation time was minimized to preserve accurate RH measurements. Utilizing straws instead of embedding sensors directly in the specimen was motivated by the intent to 1) protect the sensors, 2) be able to reuse the sensors, and 3) easily check and replace sensors in case of malfunction. The temperature measurement was not accounted because no appreciable hydration related temperature increase was observed, solely due to the small dimension of the specimens and the relatively high thermal conductivity of concrete. A time history of RH at the center of the specimens was obtained for each curing routine, which are shown in Fig. 4 ∼ 6. For the sealed specimens, the RH level at the center dropped relatively rapidly and reached about 69% on day 40, which is much lower than normal concrete and high performance concrete [23, 43]. This is due to the very low water/cement ratio and the low permeability of the UHPC. The water/cement ratio is only 0.2 of this UHPC, the amount of free water would decrease relatively fast as water is being drained through cement hydration and pozzalanic reaction. Furthermore, UHPCs have quite low permeability, water diffusion is thus slow and also low in magnitude. By comparing the experimental results shown in Fig 4 ∼ 6, one can observe that the center of specimen RH evaluations of the three curing regimes are quite close to each other.
4 LDPM modeling of early age UHPC behavior: Calibration and Validation

4.1 HTC Model Calibration and Validation

The material properties for the HTC model, including heat conductivity, cement hydration enthalpy, silica fume reaction enthalpy, hydration activation energy, silica fume reaction activation energy, and diffusivity activation energy, are obtained based on available literature [34, 45]. The moisture diffusion parameters and the self desiccation parameters are calibrated by humidity room curing RH measurements of 50 days and self desiccation RH measurements of 40 days, starting from casting, and validated by HR+WB curing RH measurements of 62 days of data, see Fig. 4 ∼ 6, where the ambient environment RH is also included. The simulated RH evolution agrees with those of the experimental investigations for the applied curing regimes very well. Also shown in Fig. 4 ∼ 6 are the evolutions of cement hydration degree, silica fume (SF) reaction degree, total reaction degree and aging degree for the three curing regimes. Aging degree of HR curing increases gradually and reaches about 0.81 on 60 days of age, while the aging degree under HR+WB curing reaches its asymptote, about 0.95, fairly early, around 14 days of age. One conclusion that can be drawn is that thermal activation results in a higher aging degree that also evolves with a higher rate. Fig. 7 and 8 present the spatial distribution of relative humidity and aging degree respectively on various ages with HR curing (14 days in 100% humidity room and room temperature).

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 material properties
used in the model are listed in Table 5, including hydration, silica reaction, moisture diffusion, heat diffusion parameters as well as parameters governing self desiccation.

Table 5: HTC Parameters

| Material property name [unit] | Symbol | Value  |
|-------------------------------|--------|--------|
| Density [kg/m³]               | ρ      | 2400   |
| Isobaric heat capacity [J/kg°C] | c_t   | 1100   |
| Heat conductivity [W/m°C]     | λ_t    | 5.4    |
| Cement hydration enthalpy [kJ/kg] | Q'_c  | 500    |
| Silica fume reaction enthalpy [kJ/kg] | E_ac/R | 780   |
| Hydration activation energy/R [K] | E_ac/R | 5490  |
| Silica fume reaction activation energy/R [K] | E_ac/R | 9700  |
| Diffusivity activation energy/R [K] | E_ad/R | 2700  |
| Silica fume efficiency [-]    | SF_eff | 0.9    |
| Polymerization activation energy/R [K] | E_op/R | 6000  |
| Hydration parameter [h⁻¹]     | A_c1   | 2 × 10^8 |
| Hydration parameter [-]       | A_c2   | 1 × 10^⁻⁶ |
| Hydration parameter [-]       | η_c    | 6.5    |
| Silica reaction parameter [h⁻¹] | A_s1  | 5 × 10^{14} |
| Silica reaction parameter [-] | A_s2   | 1 × 10⁻⁶ |
| Silica reaction parameter [-] | η_s    | 9.5    |
| Moisture diffusion parameter [m²/h] | D_0/c | 1 × 10⁻⁴ |
| Moisture diffusion parameter [m²/h] | D_1/c | 3.1   |
| Moisture diffusion parameter [-] | n     | 3.9    |
| Self desiccation parameter [-] | g_i   | 1.5    |
| Self desiccation parameter [-] | k_{v_g} | 0.2   |
| Self desiccation parameter [-] | k_{s_g} | 0.4   |

Figure 4: HTC simulation for sealed specimens for self desiccation study: (a) RH evolution and (b) simulated reaction degrees
Figure 5: HTC simulation under HR curing: (a) RH evolution and (b) simulated reaction degrees

Figure 6: HTC simulation under HR + WB curing: (a) RH evolution and (b) simulated reaction degrees

Figure 7: Relative humidity from HTC simulations under HR curing on (a) 3, (b) 14, and (c) 28 days of age
Figure 8: Aging degree from HTC simulations under HR curing on (a) 3, (b) 14, and (c) 28 days of age

4.2 Calibration of the LDPM - Aging Functions

The HTC model provides the spatial distribution of the aging degree (Fig. 8) which serves as input for aging functions relating mesoscale mechanical properties of LDPM. The aging functions, Eq. 6 \sim 8, 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 have to be calibrated. Aging of mechanical properties result from the changes in the microstructure are captured by the mesoscale model LDPM through its effect on the following mesoscale parameters: normal modulus, tensile strength, compressive yielding stress, transitional stress, and tensile characteristic length.

For the UHPC in this study a good agreement between experiments and simulations can be obtained by using $n_a = 7/3$, and $k_a = 22.2$ for the aging functions. All the LDPM simulations utilize a coarse-grained aggregate size in the range $2 \sim 4$ mm. In Cusatis et. al. [38, 39], it was demonstrated that, although approximated, the coarse-grained simulations provide good accuracy with a significant reduction in computational time. A complete list of all mesoscale parameters used in LDPM for all ages investigated can be viewed in Table 6, where the first column of numbers lists the asymptotic values. HR stands for 14 days in humidity room curing, WB stands for 7 days humidity room + 7 days water bath curing regime, after which for both curing routines the specimens are stored at room temperature with RH around 50%. Due to the small specimen dimensions, the spatial variability of aging degree for all investigated ages is below about 1%, see the standard deviation values for aging degree shown in Table 6. Hence, the difference in the simulation results including and excluding
spatial variability is negligible, see Fig. 12. Thus, spatially averaged aging degree and corresponding material properties are utilized for the simulated compression, splitting and bending tests. Also because the cylinders, cylindrical disks and beam specimens used in compression, Brazilian, and bending tests have similar size, the same material properties on corresponding ages are used for all the specimen types.

To ensure simulations utilizing spatially averaged material properties can represent the aging phenomena appreciably, the effect of spatial variability on each early age was also evaluated. Fig. 11 shows, for the mid-face of the 2x2 in (50.8x50.8 mm) cylinder on WB14/28 days, the spatial distribution of aging related mesoscale LDPM parameters including normal modulus, tensile strength and tensile characteristic length. A direct comparison between simulations with spatially constant (averaged) material properties and spatially variable properties as functions of local aging degree are presented in Fig. 12. For the investigated specimen geometries the differences are quite small with a maximum error in peak loads of 9%.

| Curing& Age       | Asym | HR3d | HR7d | HR14d | HR28d | WB14/28d |
|-------------------|------|------|------|-------|-------|----------|
| Ave. Aging Degree | 1    | 0.5582 | 0.7061 | 0.7762 | 0.8103 | 0.9541    |
| ± Standard Deviation [%] | ±0.008 | ±0.007 | ±0.072 | ±1.11  | ±0.007  |
| NormalModulus [MPa] | 75000 | 41865 | 52958 | 58215 | 60773 | 71558     |
| DensificationRatio [-] | 2.5  | 2.5  | 2.5  | 2.5   | 2.5   | 2.5       |
| Alpha [-]           | 0.25 | 0.25 | 0.25 | 0.25  | 0.25  | 0.25      |
| TensileStrength [-] [MPa] | 13.3 | 3.4  | 5.9  | 7.4   | 8.1   | 11.9      |
| CompressiveStrength [MPa] | 500  | 129  | 222  | 277   | 306   | 448       |
| ShearStrengthRatio [-] | 5.5  | 5.5  | 5.5  | 5.5   | 5.5   | 5.5       |
| TensileCharacteristicLength [mm] | 10.6 | 114  | 80   | 63    | 55    | 21        |
| SofteningExponent [-] | 0.28 | 0.28 | 0.28 | 0.28  | 0.28  | 0.28      |
| InitialHardeningModulusRatio [-] | 0.36 | 0.36 | 0.36 | 0.36  | 0.36  | 0.36      |
| TransitionalStrainRatio [-] | 4    | 4    | 4    | 4     | 4     | 4         |
| InitialFriction [-] | 0.0335 | 0.0335 | 0.0335 | 0.0335 | 0.0335 | 0.0335    |
| AsymptoticFriction [-] | 0    | 0    | 0    | 0     | 0     | 0         |
| TransitionalStress [MPa] | 300  | 77   | 133  | 166   | 184   | 269       |
| VolumetricDeviatoricCoupling [-] | 0    | 0    | 0    | 0     | 0     | 0         |
| DeviatoricStrainThresholdRatio [-] | 1    | 1    | 1    | 1     | 1     | 1         |
| DeviatoricDamageParameter [-] | 5    | 5    | 5    | 5     | 5     | 5         |
| FractureEnergy [J/m^2] | 12.47 | 15.97 | 26.28 | 29.47 | 30.12 | 21.21     |

Generally speaking, the age dependent LDPM 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, and unnotched beam bending tests, as well as size effect tests. A thorough discussion of age dependent size effect and fracture characteristics evolutions is included in the companion paper [preliminary ref].
Experimental as well as simulation results of beam TPB (50% notched) and unconfined cylinder compression tests can be found in Fig. 9 and Fig. 10 respectively. Fig. 9a and Fig. 10a present specimen setup and typical failure crack pattern from LDPM simulations for TPB and compression tests. In the subfigures, Fig. 9b-g and Fig. 10b-g, the simulation and experimental results on the six investigated early ages are shown. Specimen dimension measurements, ultimate strength, fracture energy, elastic modulus, and number of specimens are reported in the figures as well. The experimental curves of compression tests are modified to eliminate machine compliance by matching the elastic modulus indirectly obtained from beam bending tests, of which CMOD measurements are not affected by the machine deformation or load platen setup. The strength gain and stress-strain curve shapes from simulations match those from experiments quite well. The drop in strength from 14 days to 28 days as documented in the experiment section, however, is not captured in the simulations. After 14 days of 100% RH curing for both curing routines, the specimens are kept at room temperature and room RH of roughly 50%. The sudden cooling after removing the specimens from the hot water bath likely causes some damage which is further extended by drying shrinkage cracks. The presented HTC-LDPM early age model, on the other hand, is mainly focused on simulating early age strength gain and mechanical responses of concrete, thus drying shrinkage phenomena as well as the sudden cooling are not included at the moment.

The mesoscale fracture energy, calculated as $G_t = \ell_t \sigma_t^2 / 2E_0$, calculated based upon calibrated TPB test simulations, is listed in Table 6. Following a similar trend as observed in the experiments, the fracture energy generally increases as concrete ages. However $G_t$ could as well decrease with increasing aging degree and brittleness. Utilizing the calibrated aging parameter $n_a$ and $k_a$ for the UHPC investigated, $G_t$ increases until HR 28 days, after which it decreases as the material becomes more brittle with thermal activation. With the calibrated and validated aging functions (Eq. 6 ∼ 8), the mesoscale fracture energy, $G_t$, can be derived as a function of aging degree in the following form:

$$G_t = \lambda^{2n_a} \ell_t^\infty \sigma_t^\infty \left( \frac{k_a + 1}{\lambda} - k_a \right) \propto \lambda^{2n_a} \left( \frac{k_a + 1}{\lambda} - k_a \right)$$

Mathematically, $G_t$ can reach a maximum depending on $n_a$ and $k_a$, which, as aforementioned, are positive constants and can be obtained based on material properties evolutions. On the other hand, the associated tensile characteristic length decreases monotonously as aging degree goes up. This indicates a decreasing fracture process zone size while concrete ages, which is consistent with the results published in the literature
A detailed discussion of age dependent fracture properties and size effect can be found in the companion paper [preliminary ref].

Table 7 summarizes experimental as well as simulated nominal splitting tensile strengths with standard deviations for $3 \times 1$ in ($76.2 \times 25.4$ mm) circular disks. Three specimens with different discrete particle configuration are used in the simulations for each age. The experimental peak strengths don’t quite follow the expected aging trend, which leads to a certain discrepancy when compared to the strength from aging-functions-based simulations. The reason most likely lies in the experimental procedure. Unlike compression and bending tests which have constant loading rates for every test, the loading of the Brazilian tests was governed by attempts to achieve stable post-peak. Thus, force and CMOD control of different rates had to be combined manually with different switching points depending on the age-dependent brittleness of the specimen, which adds variability to the tests. In addition, the boundary conditions in the experimental setup change during the test as the top and bottom circular edge in contact with the loading blocks experience significant deformation under the applied load. This occurrence is typically difficult to model numerically.

The 1 in ($25.4$ mm) cube compression tests (Fig. 13) and unnotched $1 \times 1 \times 5$ in ($25.4 \times 25.4 \times 127$ mm) beam TPB (Fig. 14) tests are all conducted with 28 days old specimens, which were cured 7 days in the humidity room, 7 days in hot water bath, and then in air for the remaining 14 days. The nominal peak strengths of the unnotched beam bending test simulations lie within the experimental scatter, see Fig. 14b. Brittle failure in simulations also well represent that observed in the experiments. Specimen setup, crack pattern, and failure type are presented in the subfigures (Fig. 13b & 14a). For TPB simulations, note that the middle section of the beam, with its length roughly equal to its height, is lattice discrete particle model generated, while the rest of the specimen is generated as finite element mesh. This configuration is utilized both in notched and unnotched TPB simulations, see Fig. 9 and Fig. 14. This setup can save computation time, since the material in those sections stays elastic. To compare to the 3 in disks’ splitting tensile strength eliminating size effect, untouched TPB simulations were also ran using a $3 \times 1 \times 15$ in ($76.2 \times 25.4 \times 381$ mm = height $\times$ width $\times$ length) beam for HR+WB curing 14 days of age. The modulus of rupture is 14 MPa, versus experimental splitting tensile strength of 11.4 MPa. Hence, the difference between the experimental and simulated splitting tensile strengths for later ages is due to inconsistent control in the experiment and the difficulties in simulating the boundary conditions. As of the cube compression test, the simulations match the experimental data perfectly, as shown
in Fig. 13a.
Figure 9: LDPM simulations and experimental results for three-point-bend tests (a) LDPM modeling (b) HR 3 days (c) HR 7 days (d) HR 14 days (e) HR 28 days (f) WB 14 days (g) WB 28 days
Figure 10: LDPM simulations and experimental results for compression tests (a) LDPM modeling (b) HR 3 days (c) HR 7 days (d) HR 14 days (e) HR 28 days (f) WB 14 days (g) WB 28 days
Figure 11: Spatial fields of mesoscale LDPM parameters: (a) normal modulus, (b) tensile characteristic length, and (c) tensile strength, on 28 days of age under humidity room (HR) curing.

Figure 12: LDPM simulations with and without spatial variability for compression tests.

Table 7: Brazilian Tensile Strength

| Age   | HR3  | HR7   | HR14  | HR28  | WB14  | WB28  |
|-------|------|-------|-------|-------|-------|-------|
| Experiment [MPa] | 4.5  | 5.2   | 5.5   | 4.6   | 11.4  | 9.4   |
|       | ± 10.4 % | ± 9.1 % | ± 0 % | ± 19.1 % | ± 22.7 % | ± 12.2 % |
| Simulation [MPa] | 3.9 | 6.1   | 6.9   | 7.2   | 7.3   | 7.3   |
|       | ± 3.5 % | ± 3 %   | ±3.4 % | ±3.3 % | ±3 %   | ±3%    |
5 Summary and Conclusions

In recent years ultra high performance concretes have shown not only a significant rise in popularity but also practical relevance. Yet, a thorough understanding of the evolution of material properties at early age is still lacking in spite of its significance for structural design. In this paper a comprehensive numerical and experimental investigation of the early age behavior of a typical UHPC is presented. The study is based on a
large experimental campaign entailing uniaxial compression tests, tensile splitting tests, and three point bending tests at different ages and following different curing protocols, complemented by measurements of the evolution of internal humidity as indicator in sealed and unsealed samples.

In order to shed light on the evolution of macroscopic material properties, an early age model, labeled A-LDPM, is formulated within the framework of mesoscale discrete element models. The coupled processes of moisture transport, heat transfer, cement hydration, and silica fume reaction are captured by a hygro-thermo-chemical (HTC) model yielding reaction degrees and temperature corrected effective aging degree describing the local maturity of the UHPC. The local mesoscale material properties of the constitutive model, the Lattice Discrete Particle Model (LDPM), are obtained through rather simple aging functions, formulated in terms of effective aging degree.

Based on the experimental characterization clear trends in the evolution of material properties, namely unconfined compressive strength, tensile splitting strength, flexural strength as well as elastic modulus for the investigated UHPC are noted. These trends are distorted by some of the investigated curing protocol. In particular, the thermal activation in the hot water bath not only accelerated the curing but likely also had adverse affects on the material properties stemming from damage associated with the rapid cooling phase. Additional distortions in the trends may be attributed to shrinkage damage.

Utilizing the proposed computational A-LDPM framework the following conclusions can be drawn:

• The maturity of concrete can be predicted accurately if the coupled processes of moisture diffusion, heat transfer, and chemical reactions are captured in a suitable hygro-thermo-chemical framework, taking into account the environmental boundary conditions during curing.

• The effective aging degree $\lambda$ is a suitable parameter to quantify the maturity of concretes arising from cement hydration and silica-fume reaction, even following different temperature evolutions.

• By means of A-LDPM analysis of the investigated UHPC the previously postulated linear dependence of local mesoscale normal modulus on aging degree is confirmed.

• The evolution of local mesoscale strength-related parameters can be predicted well by monotonously increasing power-law type functions, formulated in terms of concrete aging degree.

• Fracture energy may exhibit a non-monotonous relationship with the maturity of concrete as documented

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in the literature for several high performance concretes and for the UHPC investigated in this study. The reason is that according to Hillerborg the fracture energy is dependent on modulus and tensile strength which may evolve at different rates. Thus, fracture energy is clearly not a basic material parameter and not suitable for the formulation of aging laws.

- Contrary to fracture energy the tensile characteristic length grows monotonously in all investigated cases and shows a linear dependence on aging degree for the studied UHPC.

- The A-LDPM framework already provides all information necessary to drive models for drying shrinkage and creep, namely the humidity rate field, the temperature rate field, and the aging degree field.

The proposed computational A-LDPM framework can accurately capture the age-dependent mechanical response of the UHPC investigated. Utilizing this framework the age-dependence of fracture characteristics and size effect are investigated in a companion paper [preliminary ref]. Future work includes the extension to and validation by normal strength concretes, and the coupling with creep and shrinkage. This extended A-LDPM framework will give access to a more substantial inverse analysis of existing datasets and allow unrivaled insights into the life-time performance of concrete structures loaded and exposed to the environment at early age.

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