Age-Dependent Lattice Discrete Particle Model for Quasi-Static Simulations

Roman Wendner, Krešimir Ninčević, Ioannis Boumakis, Lin Wan

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Age-dependent Lattice Discrete Particle Model for quasi-static Simulations

WENDNER Roman[1, a *], NINCEVIC Kresimir[1,b], BOUMAKIS Ioannis[1,c] and WAN Lin[1,d]

[1] Christian Doppler Laboratory, IKI, BOKU, Peter-Jordanstr 82, 1190 Vienna, Austria

[1,a]*roman.wendner@boku.ac.at ; [1,b]kresimir.nincevic@boku.ac.at ; [1,c]ioannis.boumakis@boku.ac.at; [1,d]linWan2012@u.northwestern.edu

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Abstract. For decades, concrete plays an important role worldwide as a structural material. Construction planning and reliability assessment require a thorough insight of the effects that determine concrete lifetime evolution. This study shows the experimental characterization as well as the results of subsequent aging simulations utilizing and coupling a Hygro-thermo-chemical (HTC) model and the Lattice Discrete Particle Model (LDPM) with aging effects for concretes at various early ages. The HTC component of the computational framework allows taking into account any form of environmental curing conditions as well as known material constituents and predicts the level of concrete maturity. Mechanical response and damage are captured by the well-established LDPM, which is formulated in the framework of discrete meso-scale constitutive models. The chemo-mechanical coupling is accomplished by a set of aging functions that link the meso-scale material properties to an effective aging degree, accounting for cement hydration, silica fume reaction, polymerization, and temperature effects. After introducing the formulations the framework is applied to experimental data of 3 standard low and higher strength concretes. Investigated tests include two types of unconfined compression, Brazilian splitting, three-point-bending, and wedge splitting. Following the model calibration the framework is validated by purely predictive simulations of structural level experimental data obtained at different ages for the same concretes.

Introduction

Nowadays, in the modern world, concrete plays a major role as a structural material and is inseparably linked to a significant part of our infrastructure. Concrete is used more than any other manmade material in the world. The behavior of a concrete structure is determined by the properties of each involved material (e.g. steel, fibers). The role of concrete is decisive, since it exhibits large statistical and spatial variability and time-dependent effects. Consequently, it is mandatory to have knowledge about the development of its mechanical characteristics as well as time dependent properties. Considering the standards, concrete structures are designed for a life span of at least 50 years. In order to ensure sufficiently high safety during the full intended life-time in a sustainable way without wasting resources accurate prediction models for time-dependent effects are quintessential.

As it is well known, concrete is an aging composite material, characterized by ongoing chemical reactions (hydration) which are dependent on the environmental conditions. As a consequence, time dependent phenomena occur during the life span of a structural element. The development of creep and shrinkage deformations on one side but also the positive development of material properties (strength and modulus) should be known over a sufficient time period in order to guarantee a safe and sustainable design of our infrastructure. Consequently, due to generally restricted testing durations it is necessary to build predictive models which include all time-dependent phenomena in concrete. Numerical models need to be calibrated by a certain number of experimental tests to ensure an acceptable quality of the required extrapolations.

The evolution of the above listed mechanical properties of concrete was investigated in this study. Further measurements include the evolution of internal relative humidity and temperature under given environmental conditions. As essential input information for numerical modelling attempts also the hydration energy was determined by a differential-calorimeter test. The internal humidity and temperature evolution is measured in three cubes of 20 cm edge length. The generated data was used in order to calibrate a hygro-thermal-chemical model (HTC) [1, 2] in order to investigate the advanced problem of curing degree related mechanical properties. The link between the HTC model and the mechanical constitutive equations are represented by a set of aging equations. This framework for the chemo-mechanical coupling is at the center of this investigation, for more see at [3, 4]. The mechanical behavior is captured by the Lattice Discrete Particle Model (LDPM) [5, 6], a well established constitutive model that is formulated in the framework of discrete elements.

The HTC component of the computational framework allows taking into account any form of curing conditions as well as known material constituents and predicts the level of concrete aging. The LDPM component simulates the failure behavior of concrete at the coarse aggregate mesoscale level and can be used to simulate the mechanical behavior of concrete structures loaded on the macroscopic level.

Numerical approaches for characterize aging

In the present paper two main components have been used to numerically model the coupled problem of chemical reaction, humidity transport and heat transfer on one side and the mechanical problem on the other side in order to ultimately predict the local curing level dependent material properties.

Hygro-Thermo-Chemical (HTC) model

The hydration process, especially in the early age, can be assumed to be the main cause of many time-dependent phenomena in concrete. The mechanical properties of concrete such as compressive and tensile strength, Young's modulus and fracture energy are closely related to the hydration degree. Furthermore hydration has a major impact on time dependent properties such as shrinkage and creep. During the reaction of water with cement (hydration), water is consumed and a volume decrease is caused. This phenomenon is called autogenous shrinkage. Additionally, drying shrinkage is caused due to drying related water loss. The hydration process is affected by the environmental conditions such as temperature and humidity which affect the availability of water for the ongoing chemical reaction as well as the reaction kinetics. Early age shrinkage and thermal strains are especially important for large concrete structures.

In order to capture the complexity and interaction of all relevant phenomena, which affect aging a numerical framework is needed. The HTC model [1, 2] is a model which is able to capture moisture transport, heat transfer and the ongoing chemical reactions. The different phenomena, which lead to aging are taken into account by mass and heat balance equations, equations describing chemical reactions and coupled transport equations. The results are reaction degrees, aging degrees and evolution of humidity and temperature. Evolution of humidity and temperature is given with the following equations:

$$\nabla \cdot (D_h \nabla h) - \frac{\partial w_e}{\partial h}\frac{\partial h}{\partial t} - \frac{\partial w_e}{\partial \alpha_c}\dot{\alpha_c} - \frac{\partial w_e}{\partial \alpha_s}\dot{\alpha_s} - \dot{w_n} = 0 \qquad (1)$$

$$\nabla \cdot (\lambda \nabla \mathrm{T}) - \rho c_t \frac{\partial T}{\partial t} + \dot{\alpha_c} c \widetilde{Q_c^\infty} + \dot{\alpha_s} s \widetilde{Q_s^\infty} = 0 \qquad (2)$$

where D_h permeability, w_e evaporable water, α_c and α_s hydration and silica fume reaction degrees respectively, w_n non-evaporable water, ρ concrete density, c_t isobaric heat capacity, λ_t heat conductivity, c and s, cement and silica fume content, $\widetilde{Q_c^\infty}$ and $\widetilde{Q_s^\infty}$ cement hydration and silica fume reaction enthalpies, respectively. Aging degree λ is typically used and formulated as:

$$\dot{\lambda} = \left(\frac{T_{max} - T}{T_{max} - T_{ref}}\right)^{n_T} \cdot \left(2A_f\alpha + B_f\right) \cdot \dot{\alpha} \qquad (3)$$

where B_f, n_T , and A_f are model parameters obtained from fitting experimental data, and α is the overall degree of reaction. The maximum temperature, T_{max}, usually is taken as 100°C, while T_{ref} is the reference temperature of mechanical tests used for the calibration of aging degree parameters.

The hygro-thermal-chemical model is formulated using the Finite Element method with an implicit solver.

Lattice Discrete Particle Model (LDPM)

LDPM [5, 6] presents a suitable discrete model to simulate the systems governed by the concrete failure modes and simulates concrete at meso-scale. Coarse aggregates are assumed to be spherically shaped in this model and are enclosed in a cementitious matrix. The connection of the aggregate centers is obtained by Delaunay tetrahedralization. The utilization of boundary conditions is ensured by randomly placed zero-radius aggregate pieces over the surfaces. The full description of the LDPM geometry is reported in [5, 6]. Taking into account that concrete ages, the local meso-scale (LDPM) material properties change and can be formulated as functions of the aging degree. In this contribution we investigate the applicability of the set of aging functions that was developed for ultra high performance concretes modelled with the same computational framework by Wan et al. [7].

$$E_0 = E_0^\infty \lambda \qquad (4)$$
$$\sigma_t = \sigma_t^\infty \lambda^{n_a} \; ; \; \sigma_c = \sigma_c^\infty \lambda^{n_a} \; ; \; \sigma_{N0} = \sigma_N^\infty \lambda^{n_a} \qquad (5)$$
$$l_t = l_t^\infty (k_a(1 - \lambda) + 1) \qquad (6)$$

The above given eq. 4 proposes that the normal modulus E_0 has a linear relation with aging degree λ. The normal modulus is related to the elastic modulus. Eq. 5 presents tensile strength σ_t, compressive strength σ_c and transitional stress σ_{N0} expressed as a power-law type function depending on aging degree λ. The last eq. 6 proposes the tensile characteristic length l_t, to be linearly decreasing with aging degree. The tensile characteristic length l_t governs the softening behavior in tensile fracture and gives information about material brittleness. According to Hillerborg [8] the tensile characteristic length is directly related to the total fracture energy by $l_{ch} = (E \cdot G_F)/\sigma_t^2$. The mesoscale fracture energy is calculated as $G_t = l_t\sigma_t^2/2E_0$.

All above aging functions given by eq. (4-6) are formulated such that the corresponding parameters approach their asymptotic values for the aging degree λ approaching the value of 1. Consequently, the input variables become the asymptotic material properties for the fully cured state.

Experimental program and results

The experimental program was carried out to characterize three standard low strength and two high strength concretes. Especially the early age mechanical behavior is investigated. The data of the experimental program has been used to calibrate and validate the presented early age model. In order to determine mechanical properties different kinds of tests were performed including compressive strength tests for cubes and cylinders (unconfined), brazilian splitting tests, three point bending and wedge splitting tests. Apart from the mechanical tests, pull-out and shear tests on slabs with headed studs, bonded anchors and threaded bars were performed. In Table 1 and Table 2 an overview of the different tests is given. In Table 3 concrete mix design for each batch can be seen.

The concrete mixes were split into five batches due to time and storage limitations. The five batches cover two concrete strength classes; three batches for low strength concrete (A2, A3 and A4 for C25/30 concrete) and two batches (B1 and C1 for C50/60 concrete) were tested.

Tests for C25/30	Days:	Specimens/day:
Compression cylinders and three point bending	2,7,14,17,23,28,52(56),87,112,(155),172,365	3-4
Compression cubes	3,8,29,134	6
Brazilian and wedge splitting	9,29	3-4
Creep	3,9,28	4
Shrinkage	1,3,9,28	2
Pull-out/shear tests	3,8,29,134	1 slab
Temperature and humidity	0	3

Table 1 Low strength concrete tests

Tests for C50/60	Days:	Specimens/day:
Compression cylinders and three point bending	1,7,14,28	4
Compression cubes	1,7,14,28,78	3-5
Brazilian splitting	1,7,14,28	4
Creep	1,6	4
Shrinkage	1,6	2
Pull-out/shear tests	7,28,78	1 slab
Temperature and humidity	0	3

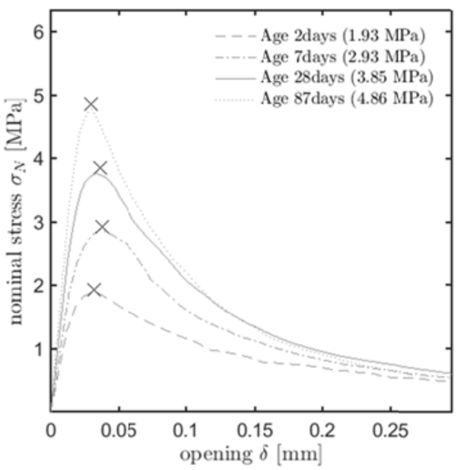
Table 2 High strength concrete tests

components	A2	A3	A4	B1	C1
cement type	CEM II 42.5 R			CEM I 52.5 R	
aggregate content [kg]	1994	1985	1979	1928	1902
cement content [kg]	242	240	237	455	464
water content [kg]	172	176	197	167	168
water/cement ratio w/c	0.71	0.73	0.83	0.37	0.36
aggregate/cement ratio a/c	8.24	8.27	8.35	4.24	4.1

Table 3 Concrete mix design

Fig. 1 shows four different nominal stress-opening curves at different ages determined by means of three point bending. It is noticed that the stiffness K as well as the peak load increase over time. The results obtained, show good quality and the curves correspond well with each other.

Fig. 2 presents the evolution of nominal bending strength from three point bending tests obtained by equation $\sigma_N = 3 \cdot F \cdot l/2 \cdot b \cdot h^2$. The solid and dashed line represent fitted aging laws suggested by EC 2. Two different approaches are considered here. First the aging law is fitted in order to get an optimized parameter s and 28 day value. The second approach uses the s value given by Eurocode for the used cement mix (CEM II: s = 0.20). It can be noticed that the obtained values for the 28 day values are similar for both approaches. The optimized fit presents an s value of 0.33 obtained with a high R^2 value of 0.92. The fixed approach gives slightly different results for the available experimental data with an R^2 of 0.81. However, the rate of strength evolution is substantially different as is the asymptotic strength. Conversely, the optimized aging law results in lower initial values and higher stresses at higher ages.



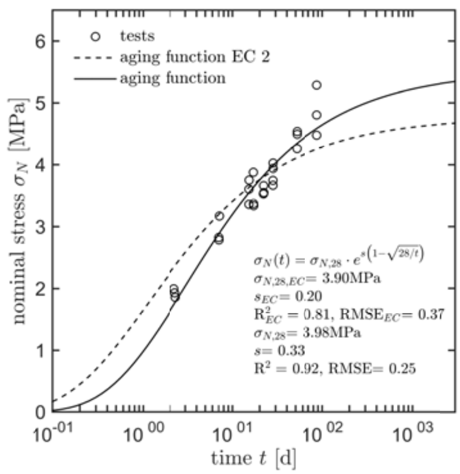
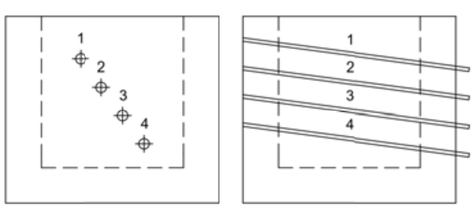


Fig. 1: Mean nominal stress-opening curves Fig. 2: Evolution of nominal bending strength

The evolution of internal humidity and temperature can be seen in Fig. 4 and Fig. 5. The sensor positions with regard to the specimen geometry are provided in Fig. 3. The data for humidity shows the expected behavior with the highest humidity for position 3 followed by position 4. Position 1 experienced the highest initial humidity, which is believed to come from a water accumulation on the top of the specimen due to a high water-cement ratio. The initial phase of hydration peaked after 1 day of curing with a maximum temperature in position 4 of around 26 degrees.



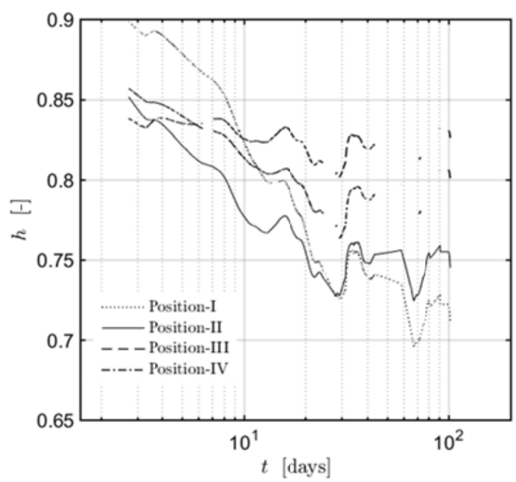


Fig. 3: Set-up for internal measurements Fig. 4: Evolution of internal humidity

The results of the hygro-thermo-chemical model calibration and experimental data for temperature evolution for low strength concrete can be seen in Fig.5 for the calibration of the low strength batch A4. For the numerical simulations of HTC model the cement hydration enthalpy has a value of 450 J/kg which has been experimentally determined using differential calorimeter test data. After the HTC model component has been calibrated by internal humidity and temperature evolution data, in the next phase the LDPM framework for the material properties calibration has to be set up. In order to validate the proposed aging functions' applicability for low to normal strength concretes, tests at different ages are first calibrated independently to then check the functional dependence of meso-scale material properties on age expressed by aging degree. This approach implies spatially uniform material properties which is not the case. Nevertheless, important insights into the behavior can be gained.

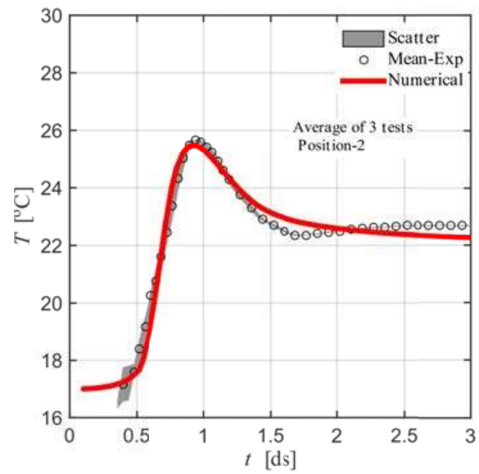


Fig. 5: Temperature evolution – experimental data and HTC model results

The calibrations have been done for three different ages (for 2, 7 and 29 days old concrete specimens) as a first approach. The calibration of LDPM parameters was completed by matching the experimentally recorded load-displacement curves for cube compression tests and load-opening curves for three point bending tests. The results of the calibrations for one low strength concrete (A4 batch) and can be seen in Fig.6 for the cube compression test and in Fig.7 for the three point bending test, both for 7 days old concrete. As can be seen in Fig.6 for cube compression tests the model has been calibrated till the peak value while in Fig.7 it can be seen that the model is able to accurately simulate also the softening behavior of the material in three point bending tests. Due to the inherent randomness in the simulated response the analysis was carried out for 5 different realizations of particle placements (seeds) each.

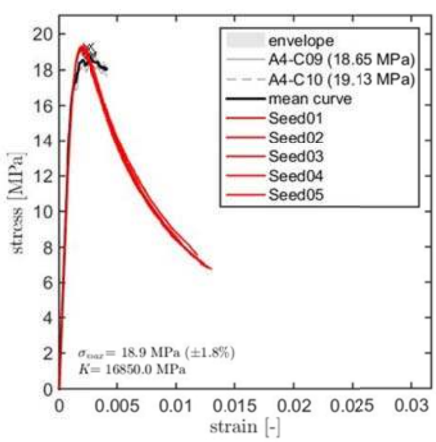


Fig. 6: Cube compression tests

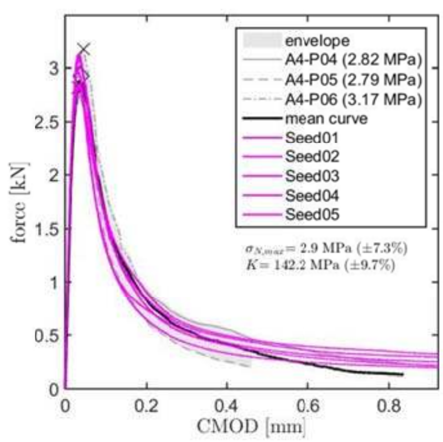


Fig. 7: Three point bending tests

In the last part of this contribution, after calibration of the HTC and LDPM models, the dependence of the meso-scale material parameters on the aging degree is investigated, starting with the set of proposed aging functions (eq.4- 6) by Wan et al. The parameters related to aging degree evolution (eq. 3), are calibrated using the compressive strength of moist cured cubes, and validated on tests of dry cured cubes, as shown in Fig. 8 and Fig. 9.

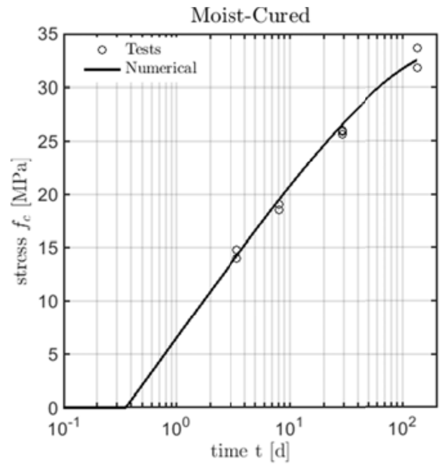


Fig. 8: Aging calibration

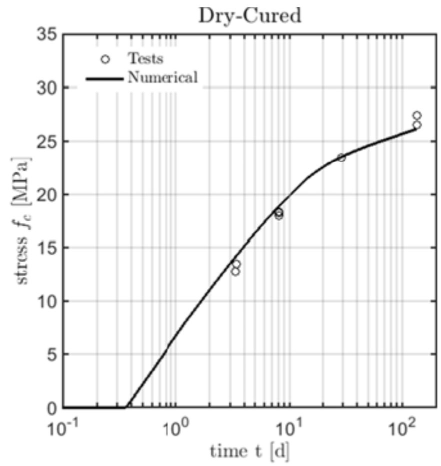


Fig. 9: Aging validation

Figures 10-13 show evolution of the meso-scale parameters, the normal modulus E_0, tensile characteristic length, l_t, shear strength ratio, and tensile strength, σ_t, depending on the aging degree λ. For the UHPC Wan et al. found a linear relationship for this parameter which is confirmed for the tensile characteristic length. Preliminary results indicate a potential linear relation also for the case of low strength concrete. The deviation for the normal modulus may be related to the actual spatial variations in modulus that have not been accounted for in the first step.

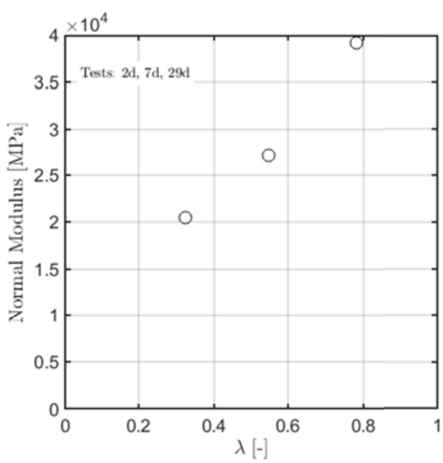


Fig. 10: Normal modulus vs aging degree

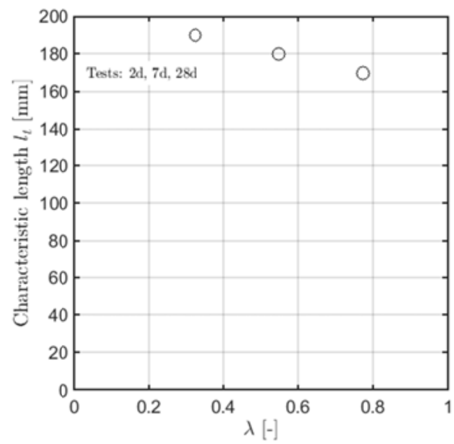


Fig. 11: Characteristic length vs aging degree

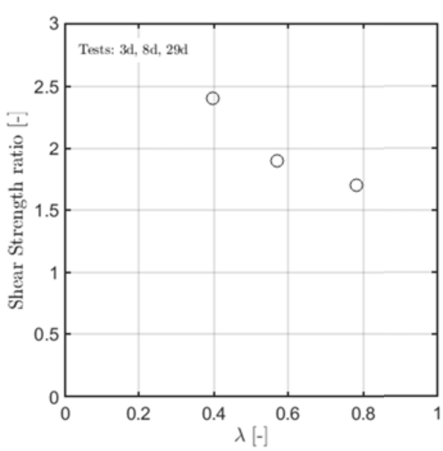


Fig. 12: Shear strength ratio vs aging degree

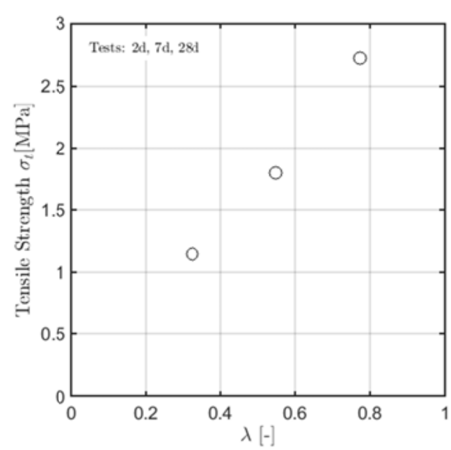


Fig. 13: Tensile strength vs aging degree

As it has already been mentioned, tensile strength σ_t, compressive strength σ_c and transitional stress σ_{N0} were proposed with power-law type relations to aging degree λ which would match the experimental data.

Conclusions

Meso-scale material properties used in the LDPM framework change while concrete ages and they can be formulated as functions of the aging degree λ. As a consequence, the evolution of the compressive and tensile strengths and moduli can be predicted in terms of the evolution of the aging degree. The logical next steps in this investigation will entail an inverse analysis running the full aging framework for all experimentally tested low strength and normal strength concretes, in order to have a wider spectrum of results for different ages. The outcome will be a set of aging functions that have been extensively validated for several different low and higher strength concretes.

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