A Parameter-Free Multiscale Framework for the Self-Desiccation in Cementitious materials

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ABSTRACT: Traditionally self-desiccation is predicted by the simulations of hygro-mechanics directly at the macro-scale providing hydration-related inputs via phenomenological constitutive models. Instead a novel method is here proposed that consists of obtaining inputs to such constitutive relations from direct simulations of cement hydration at the micro-scale using Cement Hydration in Three Dimensions (CEMHYD3D) model. This allows avoiding lengthy calibrations from experimental data. The prediction capabilities of the proposed model are demonstrated using experimental data of self-desiccation relevant to many different mix designs of concrete, mortar and cement paste, with water to cement ratios ranging from 0.20 to 0.68 and silica fume to cement ratios from 0.0 to 0.39.

1   INTRODUCTION

High and Ultra-High Performance Concrete (HPC and UHPC) have improved concrete durability in aggressive environments, and enabled the construction of complex and long-term cost-effective structures. However, these materials typically undergo self-desiccation to a significantly greater extent compared to ordinary concrete. This is due to their intrinsic mix proportions, i.e. low water to cement ratios, finer cements and addition of supplementary cementitious admixtures such as silica fume.

The term self-desiccation indicates the reduction of internal relative humidity in the pores of hydrating concrete paste. The initial water to cement ratio, the distribution of unhydrated cement particles and cement hydration chemical reactions and kinetics play a major role in self-desiccation, to cite just a few key factors. While self-desiccation may be beneficial to some extent, e.g. by enhancing resistance to internal frost damage or in concrete flooring applications, it is one of the main causes of early-age cracking, along with thermal stresses (Persson et al., 2005).

Available models in the literature can be mainly distinguished in two categories: theoretical and/or empirical formulations and direct microstructure development models. The first category encompasses mostly macro-scale models such as Hua et al. (1995), Persson (1997), and Nilsson and Mjornell (2005). Some models in the literature describe cement hydration processes, in conjunction with hygral-thermal considerations, among others Ulm and Coussy (1995), De Schutter and Taerwe (1996), Cervera et al. (1999). Among them, the Hygro-Thermo-Chemical (HTC) model proposed by Di Luzio and Cusatis (2009a,b) formulates the evolution of cement hydration and of pore relative humidity in concrete based on moisture transport and heat transfer governing equations. The model uses phenomenological evolution laws to describe the reaction degrees for cement and silica fume, and the associated changes in evaporable and chemically bound waters, along with adsorption/desorption isotherms and permeability of concrete. The HTC model is adopted in this study as the macro-scale model, which contains several material parameters to be identified on the basis of some experimental results relevant for the considered mixture that usually are not available.

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The second category of models provide a description of the actual microstructure of cement paste and concrete and reproduce directly the most important micro-scale phenomena. Among them there is the Cement Hydration in Three Dimensions (CEMHYD3D) model that was developed at the National Institute of Standards and Technology (NIST) (Bentz and Garboczi, 1990; Bentz, 1997). CEMHYD3D describes explicitly the microstructure of cement paste through a digital image based approach. Scanning Electron Microscope (SEM) images of the cement of interest are used to construct the initial 3D skeleton. Moreover, each chemical phase present in the cement powder is distinct and represented by a number of cubes/voxels that reproduce the characteristics of the SEM image, respecting the actual PSD. The model is based on a cellular automata algorithm that works through an iterative cycle process, where each voxel that constitutes a phase can dissolve, diffuse and react when in contact with other voxels.

This study, which is extensively presented in Pathirage et al. (2019), proposes a novel multi-scale approach that keeps the advantages of both modeling perspectives. Indeed, the material parameters in the macro-scale formulation are identified from the CEMHYD3D model: the relevant information is extracted and passed from lower scale to upper one. This multi-scale approach, entitled ONIX model because it requires ONly (the) mIX design as input, has the great advantage of avoiding any parameter calibration. As demonstrated in this manuscript, it allows the full prediction of self-desiccation in concrete and other cementitious composites.

2 OVERVIEW OF THE MACRO AND MICROSCALE MODELS

2.1 Macroscale formulation of self-desiccation

In the HTC model, transport phenomena in concrete are modeled at the macro-scale through two main governing equations describing heat diffusion and water transport with the temperature T and relative humidity h fields as state variables. Since this study is on self-desiccation of sealed samples, we do not consider any moisture gradient in space due to an underlying assumption of microstructural homogeneity throughout the samples at length-scales above hundred of micro-meters.

The original HTC model in the case of sealed concrete is here presented with small modifications compared to its original version to facilitate its subsequent coupling with the CEMHYD3D micro-scale evolution simulation, and to ensure that the parameter identification problem is well-posed. One can isolate a unit volume of a cementitious composite (concrete, mortar, etc.) and consider the total water content w of the isolated volume, which is a function of relative humidity, cement hydration α_c and silica fume reaction degrees α_s. The water content is given by the sum of the evaporable water w_e, which is the sum of capillary water, water vapor, adsorbed and hindered adsorbed water, and the chemically bound water w_n. The single moisture mass balance equation under isothermal and sealed conditions reads

$$\frac{\partial w}{\partial t}(h, \alpha_c, \alpha_s) = 0 \quad \text{or} \quad \frac{\partial w_e}{\partial h}\frac{\partial h}{\partial t} + \frac{\partial w_e}{\partial \alpha_c}\frac{\partial \alpha_c}{\partial t} + \frac{\partial w_e}{\partial \alpha_s}\frac{\partial \alpha_s}{\partial t} + \frac{\partial w_n}{\partial t} = 0 \quad (1)$$

In order to simulate self-desiccation in sealed conditions, one needs to impose Neumann no flow boundary conditions, along with prescribing the initial relative humidity $h = 1$ at time $t = 0$ (corresponding to initial saturation at the fresh state). For the sake of simplicity and for the small volume of materials typically considered in self-desiccation tests, the heat diffusion process can be considered fast enough for the entire process to be isothermal (T is constant).

The cement hydration degree, α_c, is defined as the ratio between the mass of cement that has reacted and its initial mass. Such a definition represents an average of the different hydration degrees associated to each individual clinker phase. The expression of its rate is based on the work of Cervera et al. (1999), and can be written as follows

$$\frac{\partial \alpha_c}{\partial t} = A_{c1}(A_{c1} + \alpha_c)\langle \alpha_c^\infty - \alpha_c \rangle e^{-\frac{\eta_c \alpha_c}{\alpha_c^\infty}} e^{-\frac{E_{ac}}{RT}} \quad (2)$$

where A_{c1}, A_{c2} and η_c are material parameters, E_{ac} is the global hydration energy and R is the universal gas constant. It is obvious that hydration degree cannot decrease in time. In order to ensure this requirement, the Macaulay brackets $\langle x \rangle = \max(0, x)$ are used. The temperature and its effect are included in the equation through an Arrhenius law. The internal relative humidity plays an important role in hydration kinetics (Powers and Brownyard, 1946; Bazant and Prasannan, 1989; Bentz, 1997). Unlike the original HTC formulation that considers the effect of relative humidity through a multiplicative factor in Equation 2, in this study, such effect is included through the value of the asymptotic degree of hydration, α_c^∞, which is assumed to decay exponentially for decreasing values of h:

$$\alpha_c^\infty(h) = \tilde{\alpha}_c^\infty e^{-\zeta_c\left(\frac{1}{h}-1\right)} \tag{3}$$

where ζ_c is a material parameter and $\tilde{\alpha}_c^\infty$ is the asymptotic hydration degree in saturated condition ($h = 1$). Finally, Equation 3 must be solved by setting $\alpha_c = 0$ at $t = 0$.

Silica fume is commonly used as a supplementary cementitious material, to generate pozzolanic reactions that involve silicon dioxide $SiO_2 = S$, in silica fume and calcium hydroxide and produce a form C-S-H, called pozzolanic C-S-H (Bentz, 2000) whose stoichiometry and specific gravity are different to those of conventional C-S-H produced by cement hydration (Cheng-Yi and Feldman, 1985). Similarly to cement hydration degree in Equation 2, one can define the silica fume reaction degree α_s as the mass of reacted silica fume particles over its initial mass. Its evolution in time can be written in a rate form as follows

$$\frac{\partial \alpha_s}{\partial t} = A_{s1}(A_{s1} + \alpha_s)\langle \alpha_s^\infty - \alpha_s \rangle e^{-\frac{\eta_s \alpha_s}{\alpha_s^\infty}} e^{-\frac{E_{as}}{RT}} \tag{4}$$

where A_{s1}, A_{s2}, η_s are material parameters and E_{as} is the silica fume reaction activation energy. Equation 4 is solved with the initial condition $\alpha_s(0) = 0$. Once again, the effect of relative humidity is taken into account through the asymptotic silica fume reaction degree α_s^∞ as

$$\alpha_s^\infty(h) = \tilde{\alpha}_s^\infty e^{-\zeta_s\left(\frac{1}{h}-1\right)} \tag{5}$$

where ζ_s is a material parameter and $\tilde{\alpha}_s^\infty$ is the asymptotic silica fume reaction degree in saturated conditions.

The rate of heat generation per unit volume due to cement hydration, $\dot{Q}_c$, is given by $\dot{Q}_c = \tilde{Q}_c^\infty c \alpha_c$ (Cervera et al., 1999). It is commonly assumed (Ulm and Coussy, 1995; Bentz and Stutzman, 1994; Cervera et al., 1999; Gawin et al., 2006) that $\tilde{Q}_c^\infty$ is constant and depends on the initial phase composition of the cement. Similarly, $\tilde{Q}_s^\infty$ represents the enthalpy of silica fume reaction per unit of reacted mass and is also assumed constant. The rate of heat generation per unit volume due to silica fume reaction, $\dot{Q}_s$, is defined as $\dot{Q}_s = \tilde{Q}_s^\infty c \alpha_s$.

It is well known that hydration degree and chemically bound water w_n can be assumed to be proportional as $w_n = \kappa_c \alpha_c c$. Where κ_c is the mass ratio of non-evaporable water at full hydration and c is the cement content. Indeed, a way to measure experimentally hydration degree is through a loss on ignition (LOI) test. One can find discordant points of view in the literature concerning the direct effect of pozzolanic reaction on the amount of non-evaporable water in the C-S-H. So here, it is here assumed as in Powers and Brownyard (1946), that the amount of reacted silica does not affect the non-evaporable water content.

To complete the description of Equation 1, one needs to provide a relationship between evaporable water, w_e, and relative humidity, h. This relationship is quantified by the adsorption/desorption isotherms. Since in environmentally sealed conditions one expects relative humidity not below 0.7-0.8, the hysteresis would be limited. So it is assumed just one single relation called sorption isotherm. The formulation implemented in the current macro-scale model is based on the phenomenological expression of Nilsson and Mjornell (2005), which explicitly takes into account the evolution of hydration and silica fume reaction, and separates the contribution of the evaporable water in the C-S-H

gel w_e^{gel} and the capillary water w_e^{cap} through $w_e = w_e^{gel} + w_e^{cap}$. The evaporable water in the C-S-H gel, determined by the so-called gel isotherm, reads as

$$w_e^{gel} = g_2 \alpha \left(c \tilde{\alpha}_c^\infty + s \tilde{\alpha}_s^\infty \frac{\tilde{Q}_s^\infty}{\tilde{Q}_c^\infty} \right) \left[1 - e^{-10 \tilde{\alpha}_c^\infty (g_1 - \alpha) h} \right] \qquad (6)$$

whereas the capillary water, or capillary isotherm, reads

$$w_e^{cap} = \frac{w_0 + \Delta w - w_n - \tilde{w}_e^{gel}}{e^{-10 \tilde{\alpha}_c^\infty (g_1 - \alpha)} - 1} \left[e^{-10 \tilde{\alpha}_c^\infty (g_1 - \alpha) h} - 1 \right] \qquad (7)$$

where g_1 and g_2 are two additional material parameters, w_0 is the initial water content, $\tilde{w}_e^{gel}$ denotes the gel isotherm at saturation, i.e. $\tilde{w}_e^{gel} = w_e^{gel}(h = 1)$. The capillary isotherm is derived from a mass balance equation and this explains the presence of the term Δw that defines the mass of water to be supplied to compensate chemical shrinkage and maintain saturated conditions. The functional form of Δw is

$$\Delta w = \kappa_{sh} \left[\left(1 - \frac{\tilde{Q}_c^\infty}{\tilde{Q}_s^\infty} \right) c \alpha_c + s \alpha_s \right] \qquad (8)$$

where κ_{sh} is a material parameter. The combination of all the previous equations allows the calculation of the relative humidity evolution in time. The numerical integration of the governing equation (Equation 1) is carried out by using a finite element approach as described by Di Luzio and Cusatis (2009b).

2.2 The micro-scale CEMHYD3D model

In order to identify the material parameters of the macro-scale model, one needs now to investigate micro-scale phenomena. CEMHYD3D generates a digitized microstructure of size 100x100x100 μm^3, made out of a cubic grid of 1 μm^3 size units called voxels, and obtained from the water to cement ratio, PSD and phase fractions of the different clinker phases and other hydration reactants. Individual cement particles are represented by a collection of voxels and are randomly placed inside the simulation box, until the target water to cement ratio and PSD are obtained. Periodic boundary conditions are imposed to avoid any boundary-related spurious effect (see Bentz and Stutzman (1994) for details regarding the algorithm).

Once the initial suspension of cement particles is created, the algorithm uses images from SEM to assign each voxel with a specific type of reactant (Bentz and Stutzman, 1994), namely C_3S, C_2S, C_3A, C_4AF, C-S-H_2 (in three forms: anhydrite CS, dihydrate C-S-H_2 and hemihydrate C-S-$H_{0:5}$), S and H. The model is now ready to *hydrate* the digitized cement paste. Hydration is simulated as a sequence of configurational changes called cycles. Each cycle involves three steps: dissolution, diffusion, and precipitation. The conversion from cycle number to time is performed through a single parameter at the end of a simulation. The relationship is a parabolic function that is written as $t_{real} = \beta n^2$ cycle where t_{real} is the real time in hours and n is the number of cycles. Different values for β (in hours/cycles^2) are reported in the literature and were obtained by calibrating the aforementioned nonlinear function against experimental data from either the evolution in time of the hydration degree or the heat release or the non-evaporable water content. In order to make ONIX a parameter-free model, the most commonly used value of the cycle to time factor, i.e. = 0:00035 hours/cycles^2 (Bentz, 1997, 2000, 2006) was selected and fixed throughout the current study.

Dissolution is represented as the conversion of a solid voxel (e.g. the above-listed hydration reactants) into one or more *packets* of diffusing species, each with size of one voxel. The dissolution implemented in CEMHYD3D is rather conceptual and simplified. All the solid voxels in the simulation box, both hydration reactants and products, are candidates for dissolution. The probability for each of them to dissolve is given by the product of three factors: solubility, a second factor that mimics the chemical kinetics of different reactions, and a third factor that is the number of first neighbor voxels, around the dissolution candidate, that pertain to the pore space.

Diffusion of species in solution is approximated as a one-step random walk of the one-voxel species within the voxels pertaining to the pore space. Each diffusing voxel is

treated independently, since in CEMHYD3D, each voxel can only be occupied by a single solid, diffusing, water or air (empty porosity) species. Once the dissolution occurs, diffusing entities corresponding to the previously listed chemical reactions proceed with a one-step random walk in the pore space available.

Table 1. Parameters of the macro-scale model to be identified.

	Parameter	Units	Identification	Value
Group 1	A_{c1}	*[1/h]*	*Calorimetric/LOI*	▯
	A_{c2}	*[-]*	*Calorimetric/LOI*	*0.005*
	η_c	*[-]*	*Calorimetric/LOI*	▯
	$\tilde{\alpha}_c^{\infty}$	*[-]*	*Calorimetric/LOI*	▯
	E_{ac}	*[kJ/mole]*	*Calorimetric/LOI*	*40.0*
	ζ_c	*[-]*	*Calorimetric/LOI*	▯
Group 2	A_{s1}	*[1/h]*	*Calorimetric/LOI*	▯
	A_{s2}	*[-]*	*Calorimetric/LOI*	*0.05*
	η_s	*[-]*	*Calorimetric/LOI*	▯
	$\tilde{\alpha}_s^{\infty}$	*[-]*	*Calorimetric/LOI*	▯
	E_{as}	*[kJ/mole]*	*Calorimetric/LOI*	*83.14*
	ζ_s	*[-]*	*Calorimetric/LOI*	▯
Group 3	κ_c	*[1/h]*	*LOI*	▯
	g_1	*[-]*	*Sorption isotherms*	*1.5*
	g_2	*[-]*	*Sorption isotherms*	▯
	κ_{sh}	*[-]*	*Geiker/Tazawa methods*	▯
	$\tilde{Q}_c^{\infty}$	*[kJ/kg]*	*Calorimetric/ Heat of solution*	▯
	$\tilde{Q}_s^{\infty}$	*[kJ/kg]*	*Calorimetric/Heat of solution*	*780.0*

LOI: Loss on Ignition, ▯: identified from the CEMHYD3D model

Precipitation can occur via three mechanisms: (1) homogeneous nucleation, where a diffusing species is directly converted into a hydration product; (2) heterogeneous precipitation, where the diffusing species can convert to hydration product only when it comes into contact with certain other solid voxels; (3) collision-based reaction, where the diffusing species can generate hydration products only upon collision with a voxel of either another specific diffusing species, or another specific solid phase. In the latter case, there are other possible chemical reactions for the diffusing species, e.g. the pozzolanic reaction. Similar to the dissolution stage, a precipitation reaction occurs with a probability that is either constant or a function of the amount of certain diffusing species in solution, to mimic the chemical kinetics of the various reactions. Finally, after a fixed number of diffusion steps (Bentz, 2000), a new cycle starts. CEMHYD3D allows for adiabatic, semi-adiabatic and isothermal conditions. In this study, only the isothermal condition is considered. Moreover, hydration can occur in either saturated or sealed conditions. In saturated condition, the pores emptied by chemical shrinkage are filled with water. In sealed condition, instead, some of the voxels corresponding to capillary pores are emptied and, to simulate near-equilibrium conditions during self-desiccation, CEMHYD3D redistributes the remaining water to ensure that the first voxels to be emptied are those pertaining to the largest still water-filled pores.

CEMHYD3D simulation provides the temporal evolution of the volume fractions of all the reactive phases and hydration products, enabling one to compute degree of hydration, chemical shrinkage, heat release rate, evaporable and chemically bound water contents, and other quantities that will be relevant for the macro-scale model.

3   BRIDGING THE TWO LENGTH SCALES: THE ONIX MODEL

3.1   Necessity of a multi-scale framework

The macro-scale model for self-desiccation introduces several material parameters that need calibration. One can classify them into three groups. Groups 1 and 2 comprise the parameters related to the two evolution laws of hydration degree and silica fume reaction degree respectively; group 3 comprises the parameters that are involved in the various constitutive relations of water phases and heats of reaction. Table 1 shows that the macro-scale model requires the calibration of 18 parameters in total. Calibrating these parameters from experiments requires at least 4 different tests: groups 1 and 2 require either adiabatic calorimetric tests to monitor the rise in temperature or the heat released, or loss on ignition tests (Bentz et al., 1997; Cervera et al., 1999; D'Aloia and Chanvillard, 2002; Nilsson and Mjornell, 2005). Group 3 requires loss on ignition tests to estimate the non-evaporable water content, but also sorption isotherms tests (Nilsson and Mjornell, 2005). Chemical shrinkage also needs to be measured separately using the methods described by Geiker (1983) or Tazawa et al. (1995). Finally, the reaction enthalpies require either measurements of heat of solution (Newman, 1950) or calorimetric tests (Livesey et al., 1991). Literature data rarely provide this whole set of measurements for a specific cement paste, and up-to-date data also happen to be scarce.

An effective way to overcome the aforementioned limitation is to determine these parameters from a micro-scale perspective. However, it is possible to keep fixed the value of some parameters (see Table 1), such as the hydration activation energy assumed as an equivalent activation energy that comprises the different activation energies of each cement powder phase (Bentz, 1997) and the activation energy of silica fume reaction (Bentz et al., 1998). The enthalpy of silica fume reaction $\tilde{Q}_s^\infty$ can be also fixed (Bentz et al., 1998). The values are identical to the ones that CEMHYD3D uses, and are assumed constant for different types of cement. Since the very first few hours of hydration are not important for practical applications and to keep the formulation simple, the parameters that control the initial part (first 24 hours) of the hydration and silica fume reaction degrees as functions of time, namely A_{c2} and A_{s2}, can also be fixed. Also the effect of the parameter g_1 involved in the sorption isotherms (Equations 10 and 11) can be assumed fixed since it cannot be obtained from the CEMHYD3D model and because its optimal value is fairly constant from data analysis of different cement composites (Di Luzio and Cusatis, 2009b). In total, 12 model parameters remain and their identification using the CEMHYD3D model is described next.

3.2   Parameter up-scaling workflow

A specific strategy is needed in order to fully take advantage of the inputs and outputs of the CEMHYD3D and the macro-scale models. Concerning the inputs, the database provides the designations of the different cements, in the case where only the type of cement is known. Further knowledge on the Blaine fineness is preferable to perform the cement selection more accurately. Once the composition is estimated, one can choose the closest cement type among the 27 available in the CEMHYD3D model database.

The first step consists in running the CEMHYD3D model at saturated condition ($h = 1$). The length of the simulation is fixed to 10,000 cycles, which represents approximately 4 years in real time, in order to capture the long-term evolution of the microstructure. Once the simulation terminates, ONIX extracts the relevant model outputs, and by keeping track of the number of voxels at each cycle and knowing the initial quantities and densities, it computes hydration degree, silica-fume reaction degree, and the evaporable water in the C-S-H gel. In addition, chemical shrinkage and heat of hydration are calculated based on the different molar volumes and heats of formation. The chemically bound water content is also estimated knowing that it is proportional to the mass of reacted clinker phases. ONIX then proceeds to an automatic parameter identification process using the non-linear least square method.

The curves of cement hydration and silica-fume reaction degrees as functions of time allow the identification of all the parameters in groups 1 and 2, with the exception of ζ_c and ζ_s, which requires a separate procedure described later. The parameters of group 3 are then determined, starting with κ_c that is identified from the non-evaporable water vs hydration degree curve. κ_{sh} is identified from the chemical shrinkage vs total reaction degree curve and g_2 from the evaporable water in the C-S-H gel vs total reaction degree curve. The latent heat of hydration, $\tilde{Q}_c^\infty$, is identified by computing the initial masses of the different clinker phases.
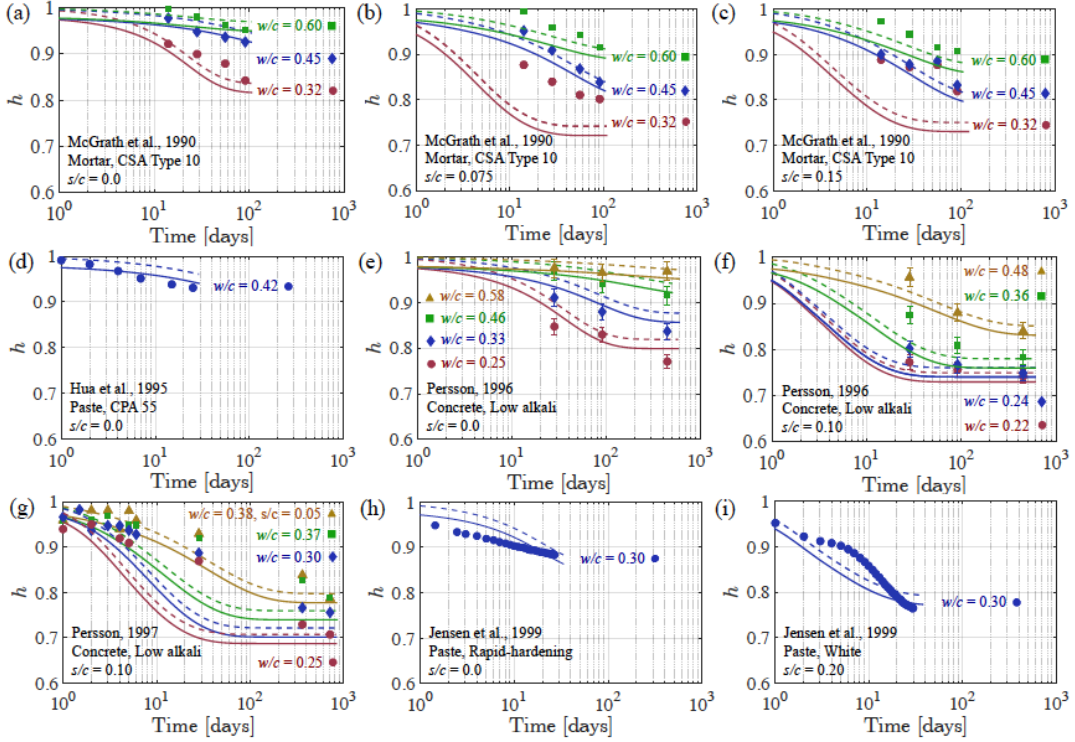

Figure 1. Prediction of self-desiccation. Markers represent experimental data, dashed and solid curves are respectively the predictions using an initial relative humidity value of $h = 1$ (upper bound) and $h = 0{:}98$ (lower bound).

At the end of this phase, the CEMHYD3D models is again used but in sealed condition for which the capillary pores are not water-filled at each cycle. This allows the identification of the latter two parameters from cement hydration and silica fume reaction degrees vs time curves respectively, which are now different from the curves corresponding to saturated conditions. The fact that the CEMHYD3D model is limited to sealed or saturated conditions does not narrow the applicability of ONIX. Indeed, the relevant parameters related to the relative humidity variation are all identified. The formulations in the HTC model then allow any external environmental conditions applied to the defined finite element domain boundaries. In the case of non-uniform relative humidity, the permeability plays of course a large role and the associated parameters are to be identified from either experimental data or from the published literature.

4   1 PARAMETER-FREE MODEL PREDICTIONS

A large collection of experimental data available in the literature is considered. The data contains self-desiccation results for 49 different cementitious composites and for all of them relative humidity was measured on sealed specimens at room temperature. Figures 1 and 2 show the full prediction results. The figures are plotted in semi-logarithm scale to highlight the long-term nature of self-desiccation. The first 24 hours are omitted due

to the lack of accuracy in the identification procedure prior to that age. The relative humidity at the beginning of the measurements reaches a plateau, at about h = 0.98 before decreasing. Typically the initial relative humidity is never h = 1 and that plateau is due to the dissolved ions in the pore solution (Lura et al., 2003). Its value depends on the water to cement ratio and on the cement composition. It may be estimated using Kelvin's equation combined with Raoult's law usually it is about $h = 0.98$. The dashed and solid curves in Figures 1 and 2 are respectively the predictions using an initial relative humidity value of h = 1 (upper bound) and h = 0.98 (lower bound). Thus, the actual prediction lies in between these two bounds and one can observe a very good agreement with the experimental data. ONIX does not explicitly take into account the mechanisms happening at a scale lower than the resolution provided by the CEMHYD3D model. Considerations of capillary depression, surface tension of colloidal particles or disjoining pressure (Hua et al., 1995) are thus only averaged.
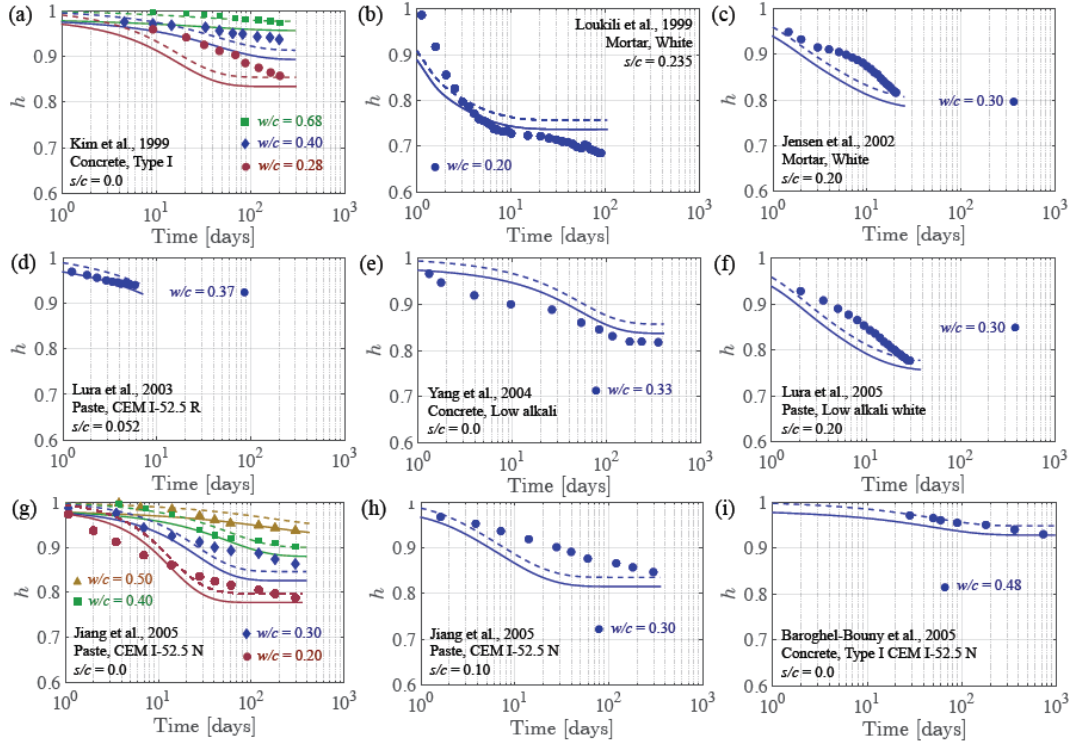

Figure 2. Prediction of self-desiccation. Markers represent experimental data, dashed and solid curves are respectively the predictions using an initial relative humidity value of h = 1 (upper bound) and h = 0:98 (lower bound).

5   SUMMARY AND CONCLUSIONS

This paper presents the formulation and validation of a novel multi-scale approach, entitled the ONIX model, to simulate self-desiccation of concrete, mortar and cement paste. The ONIX model formulates self-desiccation by means of a macro-scale mass balance equation involving evaporable water and chemically bound water whose evolution depends on the extent of the cement hydration and the silica-fume reactions. All the parameters governing the aforementioned equation are identified by using the output of micro-scale simulations carried out by the CEMHYD3D model. The ONIX model was validated by predicting self-desiccation data of different mix designs, relevant to numerous water to cement ratios, silica fume to cement ratios, cement types, Blaine finesses and cement particle size distributions.

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